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Some Applications of a New Stochastic Method

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1. INTRODUCTION

The problem is twofold here. The most outstanding problem today in the numerical study of quantum chromodynamics is to find an efficient method for treating the fermionic degrees of freedom. The problem is twofold here. The most outstanding problem today in the numerical study of quantum chromodynamics is to find an efficient method for treating the fermionic degrees of freedom. The problem is twofold here. The most outstanding problem today in the numerical study of quantum chromodynamics is to find an efficient method for treating the fermionic degrees of freedom.

ABSTRACT

Some applications of a new stochastic method to the numerical study of lattice theories...
In this so-called quenched approximation some preliminary results have been published recently\textsuperscript{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\textsuperscript{2)} which 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 which was already briefly described elsewhere\textsuperscript{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\textsuperscript{3}). Our next exercise 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

\[ S = S_0(U) + 2 \text{Re} M_{ij}(U) \bar{\eta}_j, \tag{1} \]

in four dimensions. It describes the interaction of a boson field \( U \) with a fermion field \( \eta \), and the subscripts on the fields refer to the lattice points. Spin and internal symmetry indices are suppressed, 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.
We apply the Metropolis Monte Carlo method to the evaluation of the (4)

\[ \langle n \rangle^0_s \langle n \rangle^1_s \exp\left(\text{det} \nabla \phi \right) \]

The effective action is given by

The boson-fermion system

where \( Z \) is the partition function (normalization integral) of the

(3)

\[ \langle n \rangle^0_s \langle n \rangle^1_s \exp\left(\text{det} \phi \right) \]

= 0 \quad \text{(a)} \quad \text{(b)} \quad \text{(c)} \quad \text{(d)} \]

\[ Z = \frac{\langle n \rangle^0_s \langle n \rangle^1_s \exp\left(\text{det} \phi \right)}{\text{det} \nabla \phi \}

Fermion Green's Functions

3. Fermion Green's Functions

have to refer you to some recent reviews. The fermion Green's functions can be calculated by inserting sources into the

\[ Z^{(n)} = \text{det} \nabla \phi \exp\left(\text{det} \phi \right) \]

(2)

path integral.

We will follow here the standard strategy and work directly with a new effective action, which is non-local in the presence of the fermion fields when the fermionic degrees of freedom are included.
It was shown by Scalapino and Sugar\(^{10}\), and by Fucito et al.\(^{11}\) that a local change \( U \mapsto \xi U \) implies

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

With local boson-fermion coupling the non-trivial change \( \delta M \) 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 \( (2/\mu) M^T Mx=(2/\mu) b \) where \( \mu \) is the first norm of the matrix \( M \). The driving vector \( (2/\mu) M^T b \) may be decomposed into a linear combination of unit vectors and, with the replacement \( M^T (2/\mu) M^T \), the method applies even in the worst case.

We decompose the matrix element \( H_{ik} \) into \( H_{ik}=P_{ik}+R_{ik} \), with the restriction that \( P_{ik} \geq 0 \) and \( \sum_{i=1}^{m} P_{ik}=1 \) for all values of \( i \). Consider a random walk on the domain of integers \( 1,2,\ldots,m \). 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 \( P_k=\sum_{r=1}^{k} P_{ik} \).

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 \( R_{s_{ij}} \) along the trajectory \( i=s_{1}^{\prime},s_{2}^{\prime},\ldots,s_{k}^{\prime} \) divided by the stop probability \( P_{ij} \)

\[
S_{ij} = \begin{cases} 
0 & \text{if } s_{k} \neq j \\
R_{i} R_{s_{1}} R_{s_{2}} \cdots R_{s_{k-1}} (2/\mu)^{-1} & \text{if } s_{k} = j 
\end{cases}
\] (6)
The modeling method becomes more efficient when all stop probabilities vanish. In the special case when all stop probabilities vanish, one has to stop by point \( P \). In practice, this is sometimes cheaper than \( S \). With \( S \) the decision rule, the stopping time \( S \) is \( P \), which is the stopping time of the random variable \( S \) to be smaller than \( P \). In order to compare efficiencies, we choose a simple case for illustration.

In this case, the stop probabilities vanish. The original method is equal to \( M \). The statistical errors for \( N \) walks, which all stop at point \( P \), are all positive. We now prove that the asymptotic result is the same for \( \langle S \rangle \), which is straightforward to show.

The normalizing factor is \( \lambda \). The variance of \( S \) is \( \lambda \), provided

\[
\langle S \rangle = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx
\]

where \( f_S(x) \) is the probability density function of the random variable \( S \).

It is easy to prove that the variance \( \langle S \rangle \) of the random variable \( S \) is given)

\[
\langle S \rangle = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx
\]

which is important for \( S \). The statistical error for \( N \) walks is generated by \( \langle S \rangle \). The expected value \( \langle S \rangle \) is recognized as the random variable in the decision procedure. Since

\[
\langle S \rangle = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx = \int_0^\infty f_S(x) dx
\]

we will modify the Neyman-Lijapunov algorithm for better efficiency.
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

\[
M_{ij} = -\Delta_{ij} \left( m^2 + gU_i^2 \right) \delta_{ij}
\]  \hspace{1cm} (9)

where \(U_i\) and \(\phi_i\) are a scalar boson field and a spinless fermion field, respectively. \(\Delta_{ij}\) 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 anatcically in this model, and one finds

\[
\langle i | j \rangle = \langle \phi_i \phi_j \rangle = \left( -\Delta \left( m^2 + g/2 \right) \right)_{ij}^{-1}
\]  \hspace{1cm} (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 \(D^{-1}M\). 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: \(m^2/m_r^2 = 0.78\).

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 partition function of the 2-dimensional Ising model is defined in the usual way:

\[ Z = \sum_{\text{all configurations}} e^{\beta \sum_{i,j} J_{ij} S_i S_j} \]

where \( J_{ij} \) is the coupling constant between spins \( i \) and \( j \) and \( \beta = \frac{1}{kT} \).

The two-dimensional Ising model, which was also the subject of one of our discussions here, was also known in the past to some other workers.\(^{12}\) The results of these studies are very interesting, and we are encouraged to extend the application of these methods to higher-dimensional Ising models. We note that the partition function with \( \beta = 0 \) is a special case of our results, and that for the square lattice, the partition function can be calculated exactly.

In this section we would like to discuss an interesting application of our results. The curves for the exact propagators are drawn to guide the eye. The continuous propagator of mass \( m = \frac{J}{kT} \) is the result of the numerical approximation of the propagator on the 2D lattice. When the results are extrapolated to infinite size, only a few points on a VAX 11780 to calculate the complete partition function are needed.

The speed and efficiency of the stochastic method is very promising. It took approximately 3 hours on a VAX 11780 to calculate the complete partition function.
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

$$ F = -k_B T \ln Z / N. \tag{12} $$

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\textsuperscript{13}.

We want to discuss now this connection. If the size of the lattice is $N = l \times m 
\times n$, the partition function can be written as

$$ Z = \text{Tr}(V^N), \tag{13} $$

where the transfer matrix $V$ acts on the spin states of the 2-dimensional layer of $l \times m$ sites. This slice has $2^{l \times m}$ 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 $2^{l \times m}$-dimensional, the size of the matrix $V$ is $2^{l \times m} \times 2^{l \times m}$.

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

$$ \lim_{n \rightarrow \infty} \left( \frac{\ln Z}{n} \right) = \ln \lambda. \tag{14} $$

We learn from that relation that the properties of the 3-dimensional Ising model of size $l \times m \times n$ 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

$$ V_1 = \mathbb{P}(e^{iK_z \sigma^z_{l+1}}), $$

$$ V_2 = \mathbb{P}(e^{iK_x \sigma_x^z}), $$

$$ V_3 = \mathbb{P}(e^{iH_0 \sigma^z_{l+1}}). \tag{15} $$

Here $\sigma^z$ is the Pauli spin-flip operator and $\sigma^z$ 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\textsuperscript{3}. 
The results are accurate to six decimal places. The accuracy in $F/k_B T$ is about five decimal places. The temperature dependence of the free energy is shown in Fig. 3. For fixed $T$ the results at a fixed value of $\mu$ are depicted in Fig. 2. For various lattice sizes. The values of $F/k_B T$ are depicted in Fig. 2. For various lattice sizes.

$F = \frac{k_B T}{\ln(\lambda_{max})}$
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.

![Graph showing the internal energy as a function of K](image)

**FIG. 4.** The internal energy \( U \) as a function of \( K \) for a lattice of 11x11x1 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 Grassmann 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
was done as described in section 4. We also note here that the stop probability
of the Dirac matrix along the loop. The calculation of the residues
at the initial point. For each closed random walk we calculated the
formula (6) we had to guarantee random walks which re-

determine the result above, it is possible to apply our stochastic
method to the hopping parameter expression

We apply now our stochastic method to the hopping parameter expression

The only other quantity we have to know for the calculation of composite
fermionic operators, like the current correlation function, is the matrix

When we set all the link variables to the unit matrix in Eqs. (19) and (20), we

The relativistic free fermion theory

The relativistic theory we applied the method to a free fermion gas.

In our calculation of $\Sigma$, we implemented the

and

\[ u^2 \Sigma(\eta) W_{\eta} u^2 \Sigma^{-1} = (\eta)^{\Sigma} S \]

of the two relevant quantities

\[ \det = ((\eta)^{\Sigma} S)_{\Sigma} \]

The effective fermionic action $\Sigma$ was defined in section 2 as

\[ \det W = \det W_{\eta} \]

\[ \det W_{\eta} = \det W \]

Integration over the Cremerian variables yields standard formulæ.

The last line is proportional to the hopping parameter.

The Euclidean Dirac matrices and the color SU(2) matrices connect neighbor.

\[ W_{\eta} \pi_{\eta-1} \pi_{\eta} = W \]

where $x$ is the hopping parameter and

\[ W_{\eta} = W \]

\[ 0 \]
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,

\[
S_{\text{eff}} = \sum_n C_{2n}^*(\kappa^{2n}/2n),
\]  

(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 successful ones were stored for later applications.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( C_{2n} ) (stochastic)</th>
<th>( C_{2n} ) (exact)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>((9.58 \times 0.12) \times 10^1)</td>
<td>96</td>
</tr>
<tr>
<td>6</td>
<td>((2.82 \times 0.08) \times 10^3)</td>
<td>2.82 \times 10^3</td>
</tr>
<tr>
<td>8</td>
<td>((8.30 \times 0.36) \times 10^4)</td>
<td>8.20 \times 10^4</td>
</tr>
<tr>
<td>10</td>
<td>((2.47 \times 0.25) \times 10^6)</td>
<td>2.46 \times 10^6</td>
</tr>
<tr>
<td>12</td>
<td>((7.99 \times 0.65) \times 10^7)</td>
<td>7.51 \times 10^7</td>
</tr>
<tr>
<td>14</td>
<td>((2.28 \times 1.30) \times 10^9)</td>
<td>2.30 \times 10^9</td>
</tr>
</tbody>
</table>

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 \( \kappa \) is shown in Fig. 5.

![Graph showing \( S_{\text{eff}}(\kappa) \) as a function of \( \kappa \)]

FIG. 5. The effective action \( S_{\text{eff}} \) as a function of the hopping parameter \( \kappa \) including terms from the expansion up to the 14th order. The dashed line represents the result of an exact calculation of \( S_{\text{eff}} \) on a large lattice with antiperiodic boundary condition.
In our first test runs only a few limited applications were tried so far. Since

the program is not implemented yet on the C5436 processor, we strongly

apply again to \( M \) and

Due can be repeated from time to time during long runs of the code.

are stored on disc together with their characteristic parameters. This process

are a subject of the generated loops.

At the beginning of the calculation we generate closed loops for the later

looped in the following fashion.

is implemented, the algorithm and the corresponding computer program are

the standard meteorological procedure to the updates of the gauge link

termix case, but the algorithm becomes more involved.

work vacuum polarization. This procedure remains the same as in the free

We return now to the full QCD problem in our stochastic treatment of the

Quick vacuum polarization in QCD

of the function of the inverse temperature \( T \) in dimensionless units.

The finite size dependence of the partition function, \( Z \), is depicted in Fig. 6

the free energy of the system is given by the in-

corresponds to the thermodynamics of the free relativistic quark gas of van-

for the quarks. This information is

We also made some test runs on lattices where the four-dimensional lattice was

four-dimensional volume \( V \) is depicted for the relativistic free fermion gas as

The logarithm of the partition function divided by the

particular interest in the three spatial directions and finite in the imaginary time direc-

fourth direction. The curve is shown for \( x = 0.1 \).
In order to make the thermodynamical applications more efficient and more reliable, the thermal Wilson loop \( \text{Seff} \), 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 \( \beta \).

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 \( \text{Seff} \) 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 \( 6^3 \times 3 \). 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.
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ACKNOWLEDGMENTS

Finally, we want to mention that also some other stochastic methods were re-
cently proposed for the reaction problem in QCD.

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We are indebted to P. Rujan who called our attention to the early work of

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