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THE NUMERICAL STUDY OF QUANTUM CHROMODYNAMICS[†]

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ABSTRACT

A powerful stochastic method is presented for the numerical evaluation of path integrals in quantum mechanics. The method is directly applicable for the detailed numerical study of Quantum Chromodynamics (QCD) with lattice regularization. Important results on non-perturbative physical quantities, like the confining force between a heavy quark-antiquark pair, the critical temperature of thermal quark liberation, or the mass gap for glue-ball excitations are reviewed first, within the pure gauge sector of the theory. The stochastic treatment of the complete fermionic problem is also described.

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The outline of this presentation is as follows:

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1. Introduction

After so many years there is now a general belief that we have found the theory of strong interactions as described by Quantum Chromodynamics.¹⁾ This theory is remarkably consistent with deep inelastic phenomena and provides now a consistent framework for probing hadron structures at short distances.

The great success of QCD is explained by asymptotic freedom²⁾ which tells you that the quark-gluon coupling becomes weak at short distances and perturbation theory is applicable.

On the scale of 1 fermi the coupling becomes strong, perturbation theory breaks down and the most interesting hadronic properties (mass spectrum, decay widths, wave functions, . . .) are protected from analytic calculations.

In fact, we know on quite general grounds that any hadron mass M_H depends on the bare coupling constant $g(a)$ as

$$M_H = \text{const. } a^{-1} e^{-\frac{C}{g^2(a)}} \quad (1.1)$$

which renders perturbation theory useless on the fermi scale. The space-time cut-off a at short distances carries the dimension of the mass in Eq. (1.1). It is the only dimensional quantity in the regularized theory in the limit when all quark masses vanish. The constant C in the exponent is calculable analytically, but the overall constant in front of the singular exponential function in Eq. (1.1) is not accessible by analytic methods.

The bare coupling constant $g(a)$ is a logarithmic function of the cut-off a ,

$$g(a) \sim \frac{1}{\ln \Lambda a} \quad (1.2)$$

as known from asymptotic freedom. The scale parameter Λ determines the strength of the quark-gluon coupling in QCD. Now, we note that the expression $a^{-1} \exp(-C/g^2(a))$ in Eq. (1.1) does not vary as we change the cut-off at very short distances.

Through this dimensional transmutation of Eq. (1.1) any hadron mass is of the form

$$M_H = \text{const. } \Lambda_{\overline{MS}} \quad (1.3)$$

where $\Lambda_{\overline{MS}}$ is the experimentalist's favorite scale parameter.³⁾ The constant in front of $\Lambda_{\overline{MS}}$ in Eq. (1.3) must come from a non-perturbative

calculation.

The numerical calculations I will present here strongly indicate a value around $\Lambda_{\overline{MS}} \sim 100$ MeV in the pure gluon sector of the theory, with perhaps about twenty percent uncertainty. If this value of $\Lambda_{\overline{MS}}$ will not change significantly in the presence of virtual quark vacuum polarization, SU(5) may run into trouble with the lifetime prediction⁴⁾ for proton decay,

$$\tau_p \sim 10^{32 \pm 2} \left(\frac{\Lambda_{\overline{MS}}}{\text{GeV}} \right)^4 \text{ yr.} \quad (1.4)$$

If one wants to interpret the recent underground Tata experiment in India as a lower bound,

$$\tau_p > 8 \cdot 10^{30} \text{ yr.}$$

then the situation is already becoming tight with $\Lambda_{\overline{MS}} \sim 100$ MeV.

The value of $\Lambda_{\overline{MS}}$ is only poorly known from short distance physics to be somewhere between $100 \text{ MeV} < \Lambda_{\overline{MS}} < 400 \text{ MeV}$. The main difficulty is that the predicted scaling violation effects are logarithmically slow functions of the momentum transfer. At present, experimentalists tend to prefer $\Lambda_{\overline{MS}}$ values in the lower range around 100-200 MeV.

In our numerical study of QCD we hope to determine $\Lambda_{\overline{MS}}$ accurately and less costly. We have a better chance for good accuracy, since the important relations (like Eq. (1.3)) are linear in $\Lambda_{\overline{MS}}$. It would be a great triumph to calculate the constant in Eq. (1.3) within twenty percent accuracy for the proton, the pion and other non-perturbative quantities.

The method I am going to describe is in a way an experiment. But, very importantly, it is our experiment. We, theorists, can create now interesting conditions inside the computer like the liberation of quarks at high temperature, or a container filled with glueball gas.

To understand the method, I describe it first in detail as applied to a simple quantum mechanical problem. The exciting results in Quantum Chromodynamics I will only summarize without going into details. This presentation is prepared for those who want to get a first idea about the method and who also want to see the list of results accomplished so far in Quantum Chromodynamics.

2. The stochastic method

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I will briefly describe a powerful stochastic method for the numerical evaluation of path integrals in quantum mechanics.⁵⁾ The method is easy to generalize to Quantum Chromodynamics with lattice regularization.

Consider a non-relativistic particle of mass m moving in one dimension in a potential well $V(Q)$. The particle is described by the Hamiltonian

$$H = \frac{P^2}{2m} + V(Q) \quad (2.1)$$

The transformation matrix element (transition amplitude)

$$Z_{fi} = \langle Q_f | e^{-\frac{i}{\hbar} H(t_2 - t_1)} | Q_i \rangle \quad (2.2)$$

plays a fundamental role in quantum mechanics. It describes the probability amplitude of propagation from the initial position Q_i of the particle at time t_1 to some position Q_f at time t_2 .

2a. Feynman's path integral

The time interval $t_1 - t_2$ in Eq. (2.2) can be divided into $n + 1$ segments with $t_2 - t_1 = (n + 1)\epsilon$, where ϵ is the time slice on the time lattice of Fig. 1.

Fig. 1

It is easy to show that Z_{fi} in Eq. (2.2) can be represented as the limit

of the n -dimensional integral,

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$$Z_{fi} = \lim_{n \rightarrow \infty} \int \prod_{k=1}^n \frac{dQ_k}{\left(\frac{2\pi\hbar i\epsilon}{m}\right)^{1/2}} \exp \left\{ \frac{i}{\hbar} \sum_{j=1}^n \epsilon \left[\frac{1}{2} m \frac{(Q_j - Q_{j-1})^2}{\epsilon^2} - \frac{V(Q_j) + V(Q_{j+1})}{2} \right] \right\} \quad (2.3)$$

with the notation $Q_0 = Q_i$ and $Q_{n+1} = Q_f$.

The integration over n variables in Eq. (2.3) corresponds to the sum over all zig-zag paths of Fig. 1 connecting Q_i to Q_f in the time interval $t_2 - t_1$. The limit $n \rightarrow \infty$ defines Feynman's path integral,

$$Z_{fi} = \int \left[\frac{dQ}{\left(\frac{2\pi\hbar i\epsilon}{m}\right)^{1/2}} \right] \exp \left\{ \frac{i}{\hbar} \int L(Q, \dot{Q}) dt \right\}, \quad (2.4)$$

where $L = (1/2)m\dot{Q}^2 - V(Q)$ is the Lagrangian of the particle. The transition amplitude Z_{fi} ($Q_f = Q(t_2)$, t_2 ; $Q_i = Q(t_1)$, t_1) is given by the sum of phases along all paths from Q_i to Q_f . The phase is determined by the action $S = \int L(Q, \dot{Q}) dt$ along the path.

For the numerical evaluation of the path integral we will keep n finite and work on a time lattice as depicted in Fig. 1. With sufficiently dense slicing (large n) the calculation of the path integral becomes accurate.

It is very difficult to sum the rapidly oscillating phases of the path integral, even in simple quantum mechanical applications. We follow the standard trick and rotate to Euclidean time τ with $t = i\tau$. The rotation makes real Minkowski time t now purely imaginary. In practice, this rotation corresponds to the replacement $\epsilon = ia$ in the zig-zag approximation of Eq. (2.3). The Euclidean time slice a is a small positive number on our Euclidean time lattice.

The Euclidean transformation matrix element with n moving points on the zig-zag paths is given by

$$Z_{fi}^{(n)} = \int \prod_{k=1}^n dQ_k \exp \left(-\frac{1}{\hbar} S_E(Q_i, Q_1, \dots, Q_n, Q_f) \right) \quad (2.5)$$

where we dropped the normalization factor of the integrand. It always cancels in physical quantities.

In this approximation the Euclidean action S_E is given by

$$S_E(Q_0, \dots, Q_{n+1}) = \sum_{k=1}^n \left[\frac{1}{2} m a \frac{(Q_{k+1} - Q_k)^2}{a^2} + a \frac{V(Q_{k+1}) + V(Q_k)}{2} \right] \quad (2.6)$$

and there is no integration in Eq. (2.5) over the end points $Q_0 = Q_i$ and $Q_{n+1} = Q_f$ of the Euclidean time interval.

One can study the correlation functions of the system in Euclidean time, like the two-point function

$$\frac{1}{Z_n} \cdot \int \prod_{k=1}^n dQ_k \cdot Q_1 \cdot Q_l \exp\left(-\frac{1}{\hbar} S_E(Q_1, \dots, Q_n)\right), \quad (2.7)$$

or more complicated ones. The relevant physics has to be extracted from the correlation functions.

2b. The Markov process

Feynman's path integral formulation in Euclidean time has a close analogy with a classical one-dimensional crystal. In the approximation of n integration variables, $Z_{fi}^{(n)}$ in Eq. (2.5) can be regarded as the partition function of a chain of n particles with fixed end points. There is some on-site potential energy $aV(Q_k)$ for each displacement Q_k , and there is some nearest neighbor interaction $(m/2a)(Q_{k+1} - Q_k)^2$. The energy of this classical system is given by the Euclidean action S_E . The "temperature" of the crystal is $\hbar$ formally.

Also, the Euclidean Green's functions of the original quantum mechanical problem are in one to one correspondence with the correlation functions of the one-dimensional crystal.

We want to calculate now multi-dimensional integrals of the type as in Eq. (2.7) by importance sampling of a stochastic procedure. Since the algorithm carries the awkward and misleading name of Monte Carlo method, experimentalists might get the wrong impression that they can also run this experiment.

The secret of importance sampling is that instead of throwing points into the large phase space of the n integration variables, we try to generate a distribution according to the most rapidly varying part of the integrand which is $\exp\{(-1/\hbar)S_E\}$ in our case. This is implemented through a Markov chain.

A point $(Q_1 \dots Q_n)$ in the n -dimensional configuration space represents a state of the crystal. We shall define now a stochastic process which generates new states from the initial one, step by step along a Markov chain in the state space of the system.

We start from an arbitrarily chosen point Q in the configuration space and cycle through the crystal from site to site making only a local change in the state of the crystal when we stay on a given site. On a site with some label k we generate a new value of the variable Q_k according to the probability distribution $\exp\{(-1/\hbar)S_E\}$ where all other variables are kept fixed. S_E is regarded on site k as a function of Q_k only.

This way of cycling through the lattice corresponds physically and intuitively to touching a heat bath of the right temperature $\hbar$ to

the sites of the crystal, step by step in a sequential manner. Each new state after the up-date of a site is the next element of the Markov chain.

After many sweeps we bring the crystal to thermal equilibrium at temperature $\hbar$ and the elements of the Markov chain generate now a distribution of states in configuration space according to the desired distribution $\exp\{(-1/\hbar)S_E(Q_1 \dots Q_n)\}$ in all variables.

2c. Particle in double well potential

This simple application of the above described method will demonstrate the power of the stochastic procedure. It will also help us to understand the thermodynamics of a quantum mechanical particle in a heat bath at temperature T using our formulation of the problem.

In thermodynamics the partition function of the particle is given by

$$Z = \text{Tr } e^{-\beta H}, \quad \beta = \frac{1}{kT} \quad (2.8)$$

which can be rewritten as

$$Z = \int dQ \langle Q | e^{-\beta H} | Q \rangle. \quad (2.9)$$

With the $n+1$ slices of the interval β , the end results are very similar to the propagation of a particle in Euclidean time.⁶⁾

Since we calculate the trace, there are now $n+1$ variables of integration in Eq. (2.5) where no $\hbar$ appears now. In Eq. (2.6) a is identified as $\beta/(n+1)$, and the additional variable to integrate is $Q_i = Q_f$.

We learn therefore that the thermodynamics of the quantum mechanical particle is equivalent to a periodic one-dimensional crystal, and the temperature T of the heat bath appears as $\beta = (n+1)a$ where β is the length of the crystal. It is important to distinguish between the physical heat bath which is the environment of the quantum mechanical particle in the original thermal problem and the heat bath of the stochastic procedure in generating the Markov chain. The two have nothing to do with each other.

We apply now the above described machinery to the double well potential

$$V(Q) = -\frac{1}{2}\mu^2 Q^2 + \lambda Q^4, \quad (2.10)$$

with two minima as depicted in Fig. 2. This model was studied in detail by Creutz and Freedman.

Fig. 2

When the temperature is low so that kT is much smaller than the ground state energy E_0 , we can extract information about the ground state properties of the system.

Fig. 3 shows the probability distribution of the particle in the ground state. The two maxima of the probability distribution around the potential minima is nicely seen (the next three figures are results from Creutz and Freedman⁵). The stochastic points sit on the dashed line of the exact calculation.

Fig. 3

We have a quantum mechanical tunneling problem here. The average value of the particle's position oscillates between the two potential minima for $kT \ll E_0$. This is shown in Fig. 4.

Fig. 4

With antiperiodic boundary condition, there is an instanton solution (the famous tanh function) to the classical equation of motion in Euclidean time. Creutz and Freedman find it on the one-dimensional crystal with the twisted boundary condition as depicted in Fig. 5.

Fig. 5

3. The pure gauge sector of QCD

Since we gained some confidence about the applicability of the method, it is time to turn to Quantum Chromodynamics.⁷⁾ First I will discuss the pure gauge sector of the theory.

The spirit of the calculation is the same as in the simple quantum mechanical example. The functional integrals are four-dimensional now in Euclidean space-time. We take a finite volume (box) in this 4 - d space and introduce a lattice regularization along Wilson's suggestion. Gauge fields live on links in lattice QCD and quark fields live on lattice sites.⁸⁾ We have a system with a finite number of degrees of freedom and we have to repeat a similar calculational procedure as in the simple one-dimensional example. The cut-off of the regularized theory is the lattice spacing a .

3a. String tension

The potential energy $v(r)$ between a heavy quark-antiquark pair at large separation r defines the string tension K in the pure gluon sector of the theory,

$$V(r) \sim -\frac{4}{3} \frac{\alpha(r)}{r} + Kr \quad (3.1)$$

Eq. (3.1) describes asymptotic freedom at short distances and the linear potential is associated with quark confinement. One often pictures the confining force as a chromoelectric flux tube between the quark-antiquark pair. K essentially tells you the energy per unit length stored in this flux tube.

K also relates phenomenologically to the slope $\alpha'(0)$ of Regge trajectories, if high angular momentum excitations are described as rotating strings:

$$K \approx \frac{1}{2\pi\alpha'(0)} \quad (3.2)$$

Heavy particle spectroscopy, which is based on the potential (3.1), and universal Regge slopes tend to give a value for K somewhere around

$$\sqrt{K} \approx 400 - 500 \text{ MeV}. \quad (3.3)$$

The string tension was the first physical quantity determined rather accurately by the above presented stochastic procedure. Since K is a dimensional physical quantity, it depends on the bare coupling

constant $g(a)$ as

$$K = \text{const} \cdot \frac{1}{a^2} e^{-\frac{2C}{g^2(a)}} \quad (3.4)$$

This singular behavior on the coupling constant is similar to the case of hadron masses as discussed in the introduction. The constant C is calculable in $SU(3)$, and for the sake of simplicity I did not write out a factor in front of the exponent which changes slowly as a function of g^2 . In the actual numerical calculation it is taken into account.

The results of Creutz⁹⁾ are shown in Fig. 6 for pure $SU(3)$ gauge theory. The straight line on the logarithmic plot is the envelope of the logarithm of properly chosen Wilson loop ratios to project out

Fig. 6

the coefficient of the area term ($a^2 K$) at a quark-antiquark separation l . This envelope is just $a^2 K$ for large Wilson loops, since everything is measured on the lattice in lattice spacing units.

For large bare coupling g we are in the strong coupling limit of the theory which is not physical. For very small g , the lattice spacing a becomes very small in physical units and therefore the total volume of the lattice becomes too small to pick up non-perturbative infrared effects. This is why the Wilson loops of fixed site in lattice spacing units break away from the straight line envelope.

As displayed in Fig. 6 there is only a narrow window of vulnerability where one can observe the right behavior of K as given by Eq. (3.4). In this narrow window the system follows the behavior as expected in the continuum limit $a \rightarrow 0$.

The combined results of two published calculations^{9,10)} yield a very important result

$$K^{\frac{1}{2}} = (5 \pm 2) \Lambda_{\overline{MS}} \quad (3.5)$$

in SU(3) pure gauge theory. Clearly, on the lattice one can only relate K to the strength of the quark-gluon coupling in terms of $\Lambda_{\overline{MS}}$. To find this relation also required some important calculation¹¹⁾ to connect the bare coupling constant $g(a)$ to, say, traditional regularization schemes where $\Lambda_{\overline{MS}}$ is defined.

From Eqs. (3.3) and (3.5) we estimate $\Lambda_{\overline{MS}}$ to be somewhere around 100 MeV. If this result will not change much in the presence of quark vacuum polarization, it may have interesting consequences for the proton decay in SU(5) unification.

3b. Critical temperature of thermal quark liberation

There has been a long-standing conjecture that a phase transition will take place between the low temperature confining phase of QCD and the deconfining gluon plasma phase. Quarks can move freely in the hot gluon plasma.

Recent calculations¹²⁾ give strong numerical evidence that the quark liberating phase transition occurs, indeed, in the gauge sector of QCD. The calculation goes as follows.

We insert a heavy quark-antiquark pair in the vacuum at large separation. At zero temperature some chromoelectric flux develops between the quark and antiquark and we experience a confining force law. Now we heat the system by repeating the calculation of the force at finite temperature. We saw in the case of the simple quantum mechanical example how to do the calculation at finite physical temperature.

One finds a critical temperature T_c where the confining force between the heavy quark and antiquark suddenly disappears. This phase transition is a bulk property of the system and therefore easy to detect in the calculation.

What happens somehow is that the vacuum as a medium which supported the confining chromoelectric flux gradually fills up with glueballs as the temperature is rising, and at the critical temperature T_c suddenly some gluon plasma forms. Quarks can move freely in this hot gluon plasma.

Some recent results¹³⁾ on the quark liberating phase transition are shown in Fig. 7 for SU(3). The order parameter

$$W = \exp(-\beta F) \quad (3.6)$$

where F is the free energy of an isolated heavy quark in the heat bath, is plotted against the temperature T ($\beta = 1/kT$) in some dimensionless units. We observe an abrupt change in the order parameter at the

Fig. 7

critical temperature T_c .

Below T_c the field around the isolated quark forms a collimated chromoelectric flux. Above T_c we find a Debye screened Coulomb field as shown in Fig. 8.

Fig. 8

The critical temperature T_c was found to be

$$T_c \approx \frac{\sqrt{K}}{2} \quad (3.7)$$

in the SU(3) model. The numerical value of T_c is somewhere around 200 MeV. The high energy heavy ion physics community regards the phase transition of thermal quark liberation and the low value of T_c as a real challenge.

3c. Mass gap and glueball excitations

It would be very interesting to determine numerically the mass spectrum of the lowest glueball states. Previous attempts¹⁴⁾ were based on the study of the exponential decay of correlation functions, like

$$\langle 0 | G_{\mu\nu}^2(x) G_{\mu\nu}^2(0) | 0 \rangle, \quad (3.8)$$

where $G_{\mu\nu}$ designates the field strength of the gluon field. The exponential decay of the correlation function at large separation is governed by the lowest glueball state which can be excited from the vacuum by the composite operator $G_{\mu\nu}^2$.

Recently, Wilson proposed a new improved scheme¹⁵⁾ which allows the extraction of glueball masses from correlation functions of composite operators at short distances.

The first result in the SU(3) model was recently reported¹⁶⁾ for the mass of the 0^+ glueball to be

$$m(0^+) = (2.5 \pm 0.8) \sqrt{K}. \quad (3.9)$$

The main source of the thirty percent error in Eq. (3.9) is the uncertainty in the relation between K and $\Lambda_{\overline{MS}}$ (see, Eq. (3.5)). The numerical value of the 0^+ glueball is somewhere around 1.0-1.2 GeV.

It appears that the ratio of the critical temperature T_c and the glueball mass $m(0^+)$,

$$\frac{T_c}{m(0^+)} = 0.19 \pm 0.02, \quad (3.10)$$

is very accurately known now in the SU(3) gauge model.

3d. Gluon condensate in the vacuum

The vacuum state of Quantum Chromodynamics, even in the absence of quark vacuum polarization, describes a complicated medium whose physical properties are only poorly known.

Unfortunately, we have learned only very little so far about the detailed structure of the vacuum from the numerical investigations.

We know that the vacuum as a medium is responsible for confinement, and when heated it suffers a deconfining phase transition at a critical temperature. Nothing is known about the nature of the gluon condensate which is responsible for those phenomena.

We cry for the kind of simple pictures which describe so beautifully some of the simple spin models. Fig. 9 shows the two-dimensional x-y model as it evolves and equilibrates from some configuration at $t = 0$ to a low temperature state in 1000 Monte Carlo sweeps through the lattice.¹⁷⁾ One can clearly see the Kosterlitz-Thouless vortices as they come alive from the given initial configuration when the system equilibrates in search of the important spin configurations. Of course, we know the important role of the Kosterlitz-Thouless vortices

Fig. 9

in the 2-d x-y model. The upper part of Fig. 9 describes how the system equilibrates from a hot start to some low temperature below T_c . The lower part shows the more rapid evolution from a cold start to the same equilibrium temperature.

It would be very satisfying to see that sort of qualitative insight

into the vacuum structure of QCD.

Recently we have witnessed some efforts to establish the presence of some non-perturbative gluon condensate in the QCD ground state.¹⁸⁾ The quantity

$$G = \left\langle \frac{\alpha}{\pi} \sum_{\mu, \nu, i} G_{\mu\nu}^i G_{\mu\nu}^i \right\rangle, \quad \alpha = \frac{g^2}{4\pi} \quad (3.11)$$

was extracted from Monte Carlo data for SU(2) lattice gauge theory.

In Eq. (3.11) G is the vacuum expectation value of the square of the field strength tensor $G_{\mu\nu}^i$ in Euclidean space-time metric where a summation is understood over μ, ν and the color index i .

The trace anomaly equation for the energy-momentum tensor connects G to the vacuum energy.¹⁹⁾ G is of course ultraviolet divergent with a leading term $\sim a^{-4}$ as a function of the cutoff a . To interpret G physically, the authors of Ref. 18 try to subtract from Eq. (3.11) the quantity G_{pert} which is defined as the perturbative expansion of Eq. (3.11) into a power series as a function of g^2 . The conjecture is that $G - G_{\text{pert}}$ scales under the renormalization group as an operator of dimension [mass⁴],

$$G - G_{\text{pert}} \sim \frac{1}{a^4} e^{-\frac{4c}{g^2}} \quad (3.12)$$

The subtracted expression $G - G_{\text{pert}}$ should describe then the energy decrease of the ground state in the presence of some non-perturbative gluon condensate, relative to the perturbative vacuum.

The numerical results of Monte Carlo calculations to find Eq. (3.12) as a function of g^2 are, I believe, against the above naive expectation. Two non-trivial terms are known analytically in the expansion of G_{pert} . If one includes the third term in the expansion, its unknown coefficient can be obtained from the Monte Carlo results for G in the very small g^2 region, where $G \approx G_{\text{pert}}$ to a great accuracy, according to Eq. (3.12). The difference $G - G_{\text{pert}}$, so obtained, does not scale according to Eq. (3.12) in the region $2.2 < 4/g^2 < 2.8$ which is the narrow window of vulnerability.²⁰⁾ The coefficient in the exponent is smaller by about a factor of two.

One can, of course, insist upon a fit of the form

$$G = G_{\text{pert}} + \frac{1}{a^4} e^{-\frac{4c}{g^2}} \quad (3.13)$$

to the numerical results on G by keeping many higher terms in G_{pert} with alternating signs. They cancel for very small g^2 and $G - G_{\text{pert}}$ looks good in the window. However, G_{pert} in this window does not look

like a perturbation expansion anymore. It builds up from large oscillating terms.

Clearly, one should do something better. It is difficult, if not impossible, to probe a condensate with the above method, when the natural length scale of the structure in the condensate should be of the order of 1 fermi, and not the cut-off a . Quite correspondingly, I think, it would be very difficult to see the Kosterlitz-Thouless vortices in Fig. 9 from local measurements.

4. Stochastic treatment of the fermion problem

During the last twelve months we have witnessed considerable effort to develop Monte Carlo methods for the numerical study of quantum systems with fermionic degrees of freedom. This outstanding problem is of great importance for applications in quantum field theories, condensed matter physics, and nuclear physics

Previous techniques²¹⁾ were slow when a very large number of fermionic degrees of freedom were involved, since the computational time required for a Monte Carlo sweep through the lattice was always proportional to the square of the crystal volume, or even worse.

Recently, this problem was solved by Hirsch, Scalapino, Sugar and Blankenbecker in one space and one time dimension.²²⁾ 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 is desirable.

I will follow here the more 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, a new procedure seems to maintain the efficiency of the standard Monte Carlo technique in the sense that the update time on a site is independent of the lattice volume.²³⁾ The method is applicable in any number of dimensions.

4a. Fermion determinant

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

$$S = S_0(U) + \sum_{ij} \bar{\psi}_i M_{ij}(U) \psi_j \quad (4.1)$$

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 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.

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

$$Z(\bar{\eta}, \eta) = \int D\bar{\psi} D\psi DU \exp[-S + \sum_i (\bar{\eta}_i \psi_i + \bar{\psi}_i \eta_i)] \quad (4.2)$$

By taking the functional derivatives and integrating out the Grassman variables, the fermion correlation function can be written as

$$\begin{aligned} \langle \bar{\psi}_i \psi_j \rangle &= \frac{\delta^2}{\delta \eta_i \delta \bar{\eta}_j} \ln Z(\bar{\eta}, \eta) \Big|_{\bar{\eta} = \eta = 0} \\ &= \frac{1}{Z} \int DU M_{ij}^{-1}(U) \exp[-S_{\text{eff}}(U)] \end{aligned} \quad (4.3)$$

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

The effective action is given by

$$\exp[-S_{\text{eff}}(U)] = \det[M(U)] \exp[-S_0(U)] \quad (4.4)$$

and I assume, for simplicity only, that the fermion determinant has positive sign.

I apply now the Metropolis Monte Carlo method to the evaluation of the functional integral in Eq. (4.3). Other Euclidean Green's functions can be treated similarly.

It was shown by Scalapino and Sugar²¹⁾ that a local change $U \rightarrow U + \delta U$ implies

$$\frac{\exp[-S_{\text{eff}}(U + \delta U)]}{\exp[-S_{\text{eff}}(U)]} = \det[1 + M^{-1}(U) \delta M(U)] \cdot \frac{\exp[-S_0(U + \delta U)]}{\exp[-S_0(U)]} \quad (4.5)$$

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 I 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.

I 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. It is a very efficient method for the approximate summation of the Neumann series

defined by the inverse of the operator M .

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} 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 $(2/\mu)M^+b$ may be decomposed into a linear combination of unit vectors and, with the replacement $M \rightarrow (2/\mu)M^+M$, the method applies even in the worst case.

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

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

$$S_{ij} = \begin{cases} 0 & \text{if } s_k \neq j \\ R_{is_1} R_{s_1 s_2} \dots R_{s_{k-1} s_k} P_j^{-1} & \text{if } s_k = j \end{cases} \quad (4.6)$$

I 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 $i \rightarrow j$ and to stop at j is $P(i \rightarrow j) \cdot P_j = P_{is_1} P_{s_1 s_2} \dots P_{s_{k-1} s_k} P_j$. The expected score is given by the sum over all trajectories from i to j :

$$\langle S_{ij} \rangle = \sum_{i \rightarrow j} P(i \rightarrow j) P_j S_{ij} = \sum_{i \rightarrow j} P(i \rightarrow j) R(i \rightarrow j) \quad (4.7)$$

where $R(i \rightarrow j)$ is the product of the residues along the trajectory. Since $P_{ij} \cdot R_{ij} = H_{ij}$, Eq. (4.7) is recognized as the Neumann series expansion for $M^{-1} = (I - H)^{-1}$. The term δ_{ij} in the Neumann series is generated by walks which stop immediately.

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

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

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. Therefore, the update time in this stochastic procedure is independent of the lattice volume. My tests involved matrices of the order of 10^4 , or larger.

Before we test the method on some four-dimensional fermion problem, it is appropriate to discuss a radical approximation to the fermion Monte Carlo procedure, since it was successfully applied to Quantum Chromodynamics.

4b. Hadron spectrum without internal quark loops

Recently, some very interesting results were obtained in QCD concerning chiral symmetry breaking and the spectrum of light hadrons. In the so-called quenched approximation²⁴⁾ the fermion determinant $(\det M)$ was set to one during the Monte Carlo procedure. That approximation corresponds to neglecting internal quark loops in Feynman diagrams. The hope is then that quark vacuum polarization will not play an important role in the mechanism of chiral symmetry breaking, or in the spectrum of light hadrons.

When I first studied the papers from Brookhaven²⁴⁾ I was somewhat sceptic about some of the quantitative results. Since then Claudio Rebbi kindly called my attention to some tricks they used in the numerical analysis.²⁵⁾ I assume now that the published numbers are correct within the limits of the quenched approximation.

Fig. 10

Rebbi and his co-workers find spontaneous chiral symmetry breaking in the SU(2) model with Susskind fermions. The symmetry breaking is also seen in the SU(3) model with naive lattice fermions (first paper in Ref. 24). Fig. 10 shows the non-vanishing expectation value of $\bar{\psi}\psi$ as a function of $1/g^2$ in the SU(3) model with naive lattice fermions, in the limit when the bare quark masses vanish. Quark vacuum polarization, as we said, is neglected in the calculation.

Fig. 11 shows from the first paper of Ref. 24 the light hadron spectrum as a function of the bare quark mass m_q in the SU(3) model with Wilson fermions. Very good results are reported in the absence of quark

Fig. 11

vacuum polarization, but for further details I have to refer you to the original papers.²⁴⁾

Perhaps my only somewhat sceptic remark about Fig. 11 is the very modest lattice size of $6^3 \cdot 10$ sites. The small lattice may distort to some extent the physics we want to study. I assume that results on larger lattices with accurate points will be available soon in the quenched approximation.

The effects of quark vacuum polarization remain to be seen.

4c. Method to treat the complete fermionic theory

After this excursion where $\det M$ was set to one, we return now to the complete fermion problem.²⁶⁾

I will modify now the Neumann-Ulam algorithm of Section 4a for better efficiency in fermionic Monte Carlo procedures. It is easy 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 . I define a new random variable $\tilde{S}_{ij}$ as the sum of the products of residues, adding a new term to the score at each pass through the point j . The stop probabilities are eliminated from the random variable $\tilde{S}_{ij}$, but they still govern the average length of a walk.

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

In order to compare efficiencies, I choose a simple case when all $R_{ij} = 1$ and P_j is positive. A necessary and sufficient condition for the variance of the random variable $\tilde{S}_{ij}$ to be smaller than σ_{ij}^2 is $P_j < e_j / (2 - e_j)$, where e_j designates the escape probability from the point j . In practice, this condition is enforced by the nature of the fermion problem, and the modified method is much 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 is truncated after a finite number of terms.

The modification described above is probably known to some experts on stochastic methods and the special case when the random walk is stopped by fiat appears in the Russian literature.

I tested my stochastic fermion method on a four-dimensional boson-fermion model which was first suggested by Scalapino and Sugar.²¹⁾ The fermion matrix M in Eq. (4.1) is specified now as

$$M_{ij} = -\Delta_{ij} + (m^2 + g U_i^2) \delta_{ij} \quad (4.8)$$

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 analytically in this model, and one finds

$$D(i-j) = \langle \bar{\psi}_i \psi_j \rangle = (-\Delta + m^2 + \frac{1}{2} g)_{ij}^{-1} \quad (4.9)$$

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

Some results of my calculations are presented in Fig. 12. The

complete fermion mass was generated dynamically with the choice $m = 0$. $D(i - j)$ is depicted for a lattice of $8^3 \times 16$ 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 the solid line. 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). Results are also presented for a lattice of 10^4 sites with $m_r^2 = 0.25a^{-2}$.

The quenched approximation²⁴⁾, where one neglects the fermionic vacuum polarization effects from the fermion determinant in the effective action, is also presented in Fig. 12. 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 $8^3 \times 16$ periodic lattice with $g = 2.6a^{-2}$ and $m = 0$. The contribution of the fermion loops is clearly seen and accurately calculated: $m_q^2/m_r^2 = 0.78$. In Quantum Chromodynamics I expect this ratio to be smaller.

Fig. 12

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

I hope that I can make some progress in the near future on the application of this stochastic fermion method to the numerical study of Quantum Chromodynamics.

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