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G. Parisi:
PROLEGOMENA TO ANY FUTURE COMPUTER EVALUATION OF THE QCD
MASS SPECTRUM

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PROLEGOMENA TO ANY FUTURE COMPUTER EVALUATION OF THE QCD
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I. INTRODUCTION

In recent years we have seen many computer based evaluations of the QCD mass spectrum¹. At the present moment a reliable controll of the systematic errors is not yet achieved; as far as the main sources of systematic errors are the non zero values of the lattice spacing and the finite size of the box, in which the hadrons are confined, we need to do extensive computations on lattices of different shapes in order to be able to extrapolate to zero lattice spacing and to infinite box. While it is necessary to go to larger lattices, we also need efficient algorithms in order to minimize the statistical and systematic errors and to decrease the CPU time (and the memory) used in the computation.

In these lectures the reader will find a review of the most common algorithms (with the exclusion of the application to gauge theories₂ of the hopping parameter expansion in the form I have proposed²: it can be found in Montvay's contribution to this school); the weak points of the various algorithms are discussed and, when possible, the way to improve them is suggested.

For reader convenience the basic formulae are recalled in the second section; in section third we find a discussion of finite volume effects, while the effects of a finite lattice spacing are discussed in section fourth; some techniques for fighting against the statistical errors and the critical slowing down are found in section fifth and sixth respectively. Finally the conclusions are in sections seventh.

Although these last four years have seen a great improvement of the techniques, there is still a lot to do: it would be very nice if our colleagues, which have never used a computer, would start to

study these problems, not with the aim of doing simulations themselves but for finding theoretically the best way for performing simulations: the need of better algorithms cannot be overestimated.

II. BASIC FORMULAE

In this Section the basic formulae of Euclidean field theory are recalled. Let us consider a four dimensional box of sides $L \times T$ (with periodic boundary conditions or any other kind of homogeneous boundary condition); in most of the cases we suppose $L \gg T$ and T so large that it can be practically considered to be infinite).

If only bosons are present, there is a probability measure $d\mu[A]$ (A being the generic Bosonic field) which is proportional to $\exp\{-S[A]\} d[A]$, $S[A]$ being the Euclidean action: it can be written as the integral of a local function.

If our Euclidean theory satisfies the Osterwalder Schrader axioms (which imply the existence of a corresponding Wightman type field theory in Minkowski space), we have that:

$$O_i(t) O_j(0) = \sum_n C_i^{(n)} C_j^{(n)} \exp(-E^{(n)}t) \quad (1)$$

where the operators $O_i(t)$ are functionals depending only on the A field at time t , the E_n 's are the energies of the states at rest (which are supposed to be discrete) in the Minkowski space in a box of side L . For most of the physical application we are interested to compute the E_n 's in the limit $L \rightarrow \infty$, although interesting informations on the low energy hadron-hadron interaction may be obtained if we study the L dependence.

In presence of fermionic field ($S_F = \int d^D x \bar{\psi} \Delta[A] \psi$) if C invariance is not violated, after the elimination of the Fermionic field by Gaussian integration, we remain with an effective probability distribution for the Bosonic field:

$$d\mu_F[A] = d\mu[A] \det[\Delta] \equiv d[A] \det[\Delta] \exp\{-S[A]\} \quad (2)$$

The correlation functions of the fermionic field can be evaluated easily using formulae like:

$$\begin{aligned} \langle \bar{\psi}(x) \gamma_5 \psi(x) \bar{\psi}(0) \gamma_5 \psi(0) \rangle &= \int d\mu_F[A] |G(x,0|A)|^2 \\ \Delta[A] G(x,y|A) &= \delta(x-y) \end{aligned} \quad (3)$$

Eq. 3 holds only if the bilinear operator $\bar{\psi} \gamma_5 \psi$ is not a flavour singlet, otherwise a slightly more complex formula holds.

Although the "natural" formulation of fermions is done using

anticommuting variables, only commuting quantities enter in Eqs. (2) and (3): it is possible to generate the bosonic field according to the probability distribution (2) by using a modified Monte Carlo method and the Green function $G(x,y|A)$ can be analytically computed using a fast method for solving elliptic differential equations. In the so called quenched approximation the determinant in (3) is removed: this correspond to neglect virtual quarks loops.

This program may be implemented only by introducing in the space time a mesh of size a (i.e. we consider lattice field theory): on the top of the statistical errors common to any probability based computation we have systematic errors due to the non vanishing of L^{-1} and a . Although at the end we need to do an extrapolation by considering different values of a and L , it is convenient to use algorithms which have the smallest possible systematic errors; they will be described in the next section.

III. FINITE VOLUME EFFECTS

Let us discuss firstly finite volume effects in an $SU(N)$ theory in the limit $N \rightarrow \infty$. In this case in a box of size $L \times \infty$ two phases are possible:

- a) $\langle P \rangle = 0$
- b) $\langle P \rangle \neq 0$

where P is the trace of the Wilson loop of length L winding the box. It has been argued that for $L > L_c$ $\langle P \rangle = 0$ and in this phase no physical quantity depends on L ⁵. This result is confirmed by the explicit formulae for finite volume correction written in terms of the S matrix, if we use the conjecture that the S -matrix is the identity for an $SU(\infty)$ theory.

For infinite N , $L > L_c$ would be enough for killing all the finite volume corrections. For finite N we cannot have phase transitions in a finite box and L_c is not sharply defined, however we can speak of two different regimes a) and b). In regime a) the effect of finite volume corrections may be systematically evaluated, by considering the effect of virtual particles winding through the box^{6,7}; these effects are rather small for all the virtual particles but the pion: they are proportional (roughly speaking) to

$$\exp(-mL) \tag{4}$$

Moreover the corrections to the meson spectrum are Zweig suppressed and have a small prefactor, unfortunately the corrections to the baryon spectrum are not Zweig suppressed and may be relatively high.

For boxes of reasonable size (i.e. 2 Fermi) the only effects on the masses may come from virtual pion exchange; fortunately these exchange is suppressed due to the Goldstone nature of the pion (Adler

zeros); the decoupling of the pion in this limit may be checked by computing the zero energy scattering length following Ref. 4.

At the present moment the most fashionable method for decreasing finite volume effects due to meson exchange consists in changing the masses of the quarks and to perform extrapolations to small masses¹. A more fancy possibility for reducing finite volume effects consists in playing with the boundary conditions.

In the rich men version we introduce an additional U(9) smell group: quarks transform under the fundamental representation of the group and are fermion of parastatistic 1/9; physical objects are singlet under this group; we can now impose twisted boundary conditions in the U(9) directions⁹, strongly reducing the finite volume effects. Obviously in the infinite volume limit we recover the original theory.

In the poor men version we introduce only an U(3) smell group and the boundary conditions are imposed using the following matrix diagonal in smell space¹⁰:

$$\begin{vmatrix} 1 & 0 & 0 \\ 1 & \exp(i2\pi/3) & 0 \\ 0 & 0 & \exp(i4\pi/3) \end{vmatrix} \quad (5)$$

Different quarks with different smell get different phases at the boundary: for an SU(2) theory the same prescription correspond of imposing periodic and antiperiodic boundary conditions for the two smells respectively.

The poor men version kills only the leading terms ($\exp(-m_M L)$) leaving subleading terms $\exp(-m_M \sqrt{2}L)$, while the rich version kills all terms up to $\exp(-3m_M L)$ but costs more in CPU time and memory.

The poor man version is recommended in all cases where memory and not CPU is the limiting factor while the rich man version is compulsory for studying more subtle effects like the g width.

IV. THE LATTICE SPACING

In order to perform a simulation it is necessary to introduce a lattice spacing (let us call it a).

In a pure gauge theory it was proven by Symanzik¹¹ that the finite lattice spacing corrections are proportional to a^2 and it is possible to find out an action on the lattice such that these corrections are absent: in an asymptotically free theory the action may be computed in perturbation theory in the bare coupling constant. When fermions are present the corrections are proportional to a and are much more serious.

The advantages of using an improved action have been carefully

investigated by Monte Carlo in the case of the two dimensional σ -models¹² and start to be investigated in the case of the lattice gauge theories.

In my opinion the effects of the improvement would be small for pure gauge theories (provided that we stay far away from the critical point in the β -fundamental β -adjoint plane¹²) while the improvement seem to be absolutely necessary for fermions where the effects are much stronger; careful studied in this direction would be very interesting: the field is rapidly developing and it is difficult to provided an updated list of references.

A related subject which is not yet studied is how to improve the results of a simulation done in the Langevin approach¹³ by trying to compensate the finite time step effects (in this context time is the fifth dimensional computer time) with the finite lattice spacing effects. Let us consider a trivial case: massless free field theory in one dimension. In the continuum the Langevin equation is

$$\dot{\varphi} = \Delta \varphi + \eta \overline{\eta(x_1 t) \eta(y_1 t)} = 2 \delta(x-y) \delta(t-t') \quad (6)$$

When we introduce a lattice spacing a and a time spacing ε the Langevin equation can be written as:

$$\begin{aligned} \tilde{\varphi}_n(i) &= \varphi_n(i) + R_n(i) \varepsilon^{\frac{1}{2}} & \overline{R_n(i) R_m(j)} &= \frac{2}{a} \delta_{i,j} \delta_{n,m} \\ \varphi_{n+1}(i) &= \tilde{\varphi}_n(i) + \varepsilon \left[\tilde{\varphi}_n(i+1) + \tilde{\varphi}_n(i-1) - 2 \tilde{\varphi}_n(i) \right] / (2 a^2) \end{aligned} \quad (7)$$

An easy computation in momentum space tell us that:

$$G(P) = \varphi(P) \varphi(-P) = \frac{1}{P^2 + (\frac{\varepsilon}{2} - \frac{a^2}{12}) P^4 + O(P^6)} \quad (8)$$

at the magic value $\varepsilon = a^2/6$ the effects of order a^2 cancels with those of order ε . Independently of the possibility of cancelling errors of different origins, it is clear that if the continuum limit is done at a^2/ε constant, the final errors remain of order a^2 . A more careful investigation of these problems would be welcome, also given the relevance of the Langevin equation for introducing Fermion loops.

V. FIGHTING AGAINST STATISTICAL ERRORS

Everyone would agree that if we want to measure something (e.g. $\langle O \rangle$ near the continuum limit) it is better to consider a quantity which has a definite probability distribution in the continuum limit, i.e. if $P(z)$ is the probability that $O=Z$, we would like that in the continuum limit the limiting probability $P_c(Z)$ exists and it is such that:

$$\int_{-\infty}^{+\infty} P_c(z) dz = 1 \quad (9)$$

As far as the statistical errors are proportional to $\langle O^2 \rangle - \langle O \rangle^2$ we would like that the noise to signal ratio

$$R = \frac{N^2}{S^2} = \frac{\langle O^2 \rangle}{\langle O \rangle^2} - 1 \quad (10)$$

remains finite in the continuum limit.

Unfortunately it is well known that if O is a local operator in more than one dimensions:

$$P_c(z) = 0 \quad (11)$$

Fields are not functions but distributions: only observable constructed with smeared fields have a well defined probability distribution.

If we use local operators to compute the masses the ratio noise to signal diverges in the continuum limit; e.g. if we measure the glueball mass by looking to the plaquette plaquette correlation function the noise to signal ratio diverges like a^{-16} , making the computation impossible for small a .

Generally speaking in order to compute masses it is convenient to consider observables which are functional of the field smeared in space and not in the time in order to preserve Eq. (1). This can be trivially done in a non gauge theory. In a gauge theory we have two options:

- a) we fix the gauge (i.e. the Coulomb gauge¹⁴) and we smear the gauge variables in this gauge;
- b) we use a gauge invariant construction for the block gauge field (e.g. the one proposed by Wilson restricted on a space slice). A very simple and efficient procedure is discussed in Ref. 15, as far as the computation of the glueball is concerned.

We notice en passant that all the informations on the low energy spectrum are contained in the block fields and going from the original lattice to a new lattice with twice lattice spacing we loose only informations on the high energy part of the spectrum, which is not so important; however the number of variables will decrease of a factor 8-16. The variational approach for computing the eigenvalues can be done by starting directly from the block field configurations (reducing the amount of work needed if we consider many operators); moreover we could save on a tape only the block field configurations and the block quarks propagator, strongly reducing the input-output problem.

It is also possible to decrease the statistical error¹⁶ by a careful use of the DLR equations in order to find a new observable O' such that $\langle O' \rangle = \langle O \rangle$ and $\langle (O')^2 \rangle \ll \langle O^2 \rangle$.

This procedure has been used for computing the string tension with rather good results. The most efficient way I can think to measure the string tension using the DLR identities is the following: we consider a lattice $L^3 \times T$ where all gauge fields at $t=0$ are equal to zero ($U=1$). The expectation value of the Polyakov loop P in the x direction decrease for large L as

$$\langle P(t) \rangle \approx \exp(-KLt) \quad (12)$$

The appropriate DLR identity is:

$$\langle \prod U_x \rangle = \overline{\prod \langle U_x \rangle_x} \quad (13)$$

where $\langle U_x \rangle_x$ denotes the average over the links in the x direction and the bar the average over the other links. The implementation of the identity is rather simple: we start from independent gauge field configurations and we upgrade only the field in the x direction with the other fields quenched; in this way we compute an approximate expectation value of each link U_x and the Polyakov loop is computed as the product of all the approximated expectation values. At the end we average the configurations of the gauge fields. This procedure may be also used to compute the correlation function of two Polyakov loops at distance larger than 1 if the slice at $t=0$ is not cold (i.e. $A=0$) but it is at thermal equilibrium and we quench also the values of the U_x 's on the two slices (i.e. at $t=0$ and $t=T/2$). This procedure should be used only if one is interested to compute the potential, not only the string tension; indeed it is well known that unless special techniques are used the best way for computing the exponential decay of correlation functions consists in measuring the response function¹⁷.

VI. FIGHTING AGAINST THE CRITICAL SLOWING DOWN

From the lattice point view the continuum limit is a second order phase transition at which the coherence length becomes infinite. For a theory whose Lagrangian is quadratic in the momentum it is well known that the dynamics of the low frequency modes slows down of a factor a^2 , i.e. the number of Monte Carlo interaction needed to produce independent configurations increase as a^{-2} , neglecting logarithms. The same result follows in the Langevin approach where the time step must be of order a^2 . Pictorial we could say that the information diffuses on the lattice (or makes a random walk) so that we need a time proportional to ℓ^2 in order to change the block variable associated to a region, of size ℓ , in lattice spacing units.

This slowing down should be avoided as far as possible: at my

knowledge there are two methods which solve this problem, the FFT preconditioned Langevin equation and the Multi Grid Monte Carlo.

Let us first describe the Langevin approach for a scalar field theory with action

$$S[\varphi] = \int d^d x \frac{1}{2} [(\partial_\mu \varphi)^2 + V(\varphi)] \quad (14)$$

As we have already mentioned it is well known that:

$$\langle 0[\varphi] \rangle = \overline{0[\varphi]} \quad (15)$$

where as usual the bar denotes the average over the noise and φ is the solution of the Langevin equation:

$$\dot{\varphi} = \Delta\varphi - V'(\varphi) + \eta \quad \eta(x, t) \eta(y, t') = 2\delta(t-t')\delta(x-y) \quad (16)$$

Now we would like to increase the speed of the slow variables at low momenta; a very interesting theorem tells us that equation (15) still holds if we consider the generalized Langevin equation:

$$\begin{aligned} \dot{\varphi}(x) &= \int dy Q(x-y) [\Delta(y) - V'(\varphi(y))] + \eta_Q(x) \\ \eta_Q(x, t) \eta_Q(y, t') &= 2\delta(t-t') Q(x-y) \end{aligned} \quad (17)$$

where the kernel Q has been chosen in such a way to have a fast speed up the low momentum region: e.g. $Q(x) = \int dk \exp(ikx) (k^2 + m^2)^{-1}$.

The computation of the convolution can be done in momentum space and the Fourier transform can be done using the Fast Fourier Transform algorithm which is quite efficient (the slowing down is now proportional to $\ln a$). It looks like that the best choice of $Q(x)$ consists in taking

$$Q(x) \simeq \langle \varphi(x) \varphi(0) \rangle \quad (18)$$

however this question should be investigated in a more detailed way.

The same technique may be used for gauge theories (in the Landau gauge it is likely that $Q(x)$ should behave like $\exp(-x^2)$ at large distance) if we remove the constraint that the U variables belong to the gauge group and we replace it with an appropriate weight in the action; on the other hand this method could be well used for Fermions both in the pseudofermions approach and in the computation of the Green function, using the Gauss Seidel or the conjugate gradient methods.

The basic idea of the multigrad Monte Carlo approach consists in introducing a variable for each field and also for each block field. In lattice of size $L=2^n$ we can write¹⁸

$$\varphi(i) = \sum_0^n \sum_k c_{i,j}^{(k)} \varphi^{(k)}(j),$$

where each component of the the index j runs from 1 to 2^{n-k} and the $c_i^{(k)}$ are appropriate constant.

We can now perform a Monte Carlo simulation on all the variables together; also in absence of tricks for fastening the computation, the total time for a multigrad Monte Carlo cycle will be at worse proportional to n , i.e. the algorithms is slow only of a factor $\ln a$. The benefit of the multigrad algorithm is that the efficiency for changing the low momentum variables should be quite high and no critical slowing down should be present. This may happens if the constants $C(k)$ are chosen in the appropriate way: simple minded arguments suggest that for an action with two derivatives the c 's must be linear in j while for the action with only one derivative the c 's can be constant inside each block.

The method should be particularity efficient for quadratic actions: (the CPU time for a multigrad sweep is similar to the one for an usual sweep) expecially for the computation of the Fermionic propagator which is a first order differential equation. On the contrary the application of the multigrad method to the gauge field sector seems to be particularly paintfull but it may be rewarding.

It could be very interesting to see how these methods work in a concrete case.

VII. CONCLUSIONS

I believe that in the future the methods described in the two last sections will lead to a strong reduction of the CPU time needed to perform a computation. The use of block fields for constructing the observable decreases the statistical errors; moreover as far as the block fields should excite from the vacuum only low energy particles Eq. (1) will be dominated by the lowest energy state also at moderate values of t , allowing therefore an unbiased determination of the masses of the lowing lying states. On the other hand the multigrad method should strongly fasten the slow part of the computation, i.e. the treatment of the Fermions.

It seems that we havè at our disposal all ingredients for performing a successful computation of the hadronic spectrum keeping under control the systematic errors.

At the present moment, on most of the super computers the main limitation seems to be lack of memory space; the trend is reversing: new generation supercomputers will have a reasonable amount of memory (may be not enough). With the advent of 256 kb chips also dedicated computers may be equipped with a sufficient large amount of memory. A serious problem that slows down the progress in this field is the difficulty in writing down the computer code which implements the various algorithms, i.e. the software problem. This

implements the various algorithms, i.e. the software problem. This problem becomes stronger if we want to write down efficient codes for pipelined or parallel machines. A possible way to overcome these difficulties is discussed in Wilson's contribution to this school.

Of course the final solution for decreasing the memory space (may be not the CPU time) is to push Symansik's improvement program or/and Wilson's renormalization group approach. This may be crucial especially for the properties of the pion in a realistic simulation in order of not upsetting the cancellation of virtual pion exchange due to the quasi Goldstone nature of the pion.

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- F1. It is well know that in reality the masses of the barions and the mesons contain non analytic terms like $m_q^{3/2}$ and $m_q^2 \ln m_q$ (m_q being the quark mass) with computable coefficients, moreover there are indications from the experimental value of the sigma term in pion proton scattering that strong non linearities in the barionic masses are present when the quark mass changes from the up to the strange mass. These terms should be practically absent in the quenched approximation: they are Zweigh suppressed: similar arguments suggest that the nucleon mass may be about 1100 MeV in the quenched approximation, i.e. it should be similar to the purified mass of Ref. 8.
- F2. The observed "scaling" behaviour of the gluball mass near 5.6 implies that these data are useless to conclude something on the continuum limit: indeed both the string tension and the deconfinement critical temperature do not scale in this region and the scalar glueball mass is the most sensitive quantity to the existence of the nearby critical point: it seems likely the observed "scaling" of the glueball is simple a coincidence without any deep meaning.