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Contribution to the Les Houches Meeting, March 1983.

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THE STRATEGY FOR COMPUTING THE HADRONIC MASS SPECTRUM

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1. - INTRODUCTION

In the last years many papers have been published in which spectrum and the static properties of the low lying hadrons have been computed for lattica QCD. The goal is to prove or to disprove QCD by a direct comparison of the theory with the "low" energy data. This goal can be reached only if statistical and systematic errors are under controll. In these first generation papers(1) (as it was clearly stated) the control of the systematic effects was lacking because of the relative short CPU time used and the consequential impossibility of going to larger lattices. At the present moment a second generation of computations is starting(2) and systematic effects will be careful studied.

It is clear that it is possible to plan a computer simulation in a rational way only in presence of a priori estimates of the size of the errors: systematic errors may be removed only if we understand their origine and we know the dependance of the systematic errors on the various control parameter of the simulation.

In this note we address to these problem in the framework of the quenched approximation(3), i. e. no fermion loops. There are no difficulties to remove the quenching and to introduce fermionic loops, the corresponding increase in CPU time of the computation should range from 3 to 30, for more details the reader may look to ref. (3-4).

In section 2 we discuss the estimates of the statistical errors, while in sections 3, 4, 5 and 6 we discuss the different sources of systematic errors: finite lattice spacing, finite euclidean time separation, finite volume effects and finite quark masses respectively.

2. - STATISTICAL ERRORS

The basic formula needed to estimate statistical errors is rather simple: if A is an observable and $\bar{A}^{(N)}$ is its average after N measurements (which for simplicity we suppose to be statistically uncorrelated) we know that for large N

$$\bar{A}^{(N)} = \langle A \rangle + r(\langle A^2 \rangle_c / N)^{1/2} \quad , \qquad \langle A^2 \rangle_c = \langle A^2 \rangle - \langle A \rangle^2 \tag{1}$$

where $\langle A \rangle$ is the exact expectation value and r is gaussian random number with unit variance. Eq. (1) is essentially the central limit theorem.

It is clear the we would like to have statistical errors as small as possible without having to increase N to much. This can be done if we find an observable B such that

$$\langle A \rangle = \langle B \rangle \ , \qquad \langle A^2 \rangle > \langle B^2 \rangle \, . \tag{2}$$

An elementary example of this procedure can be found in the Ising model where the Hamiltonian is

$$H = \frac{1}{2} \sum_{i,k} J_{ik} \sigma_i \sigma_k \tag{3}$$

and the σ's are variables which takes only the values ± 1.

The Callen identity[(5)] (which is a special case of the DLR equations[(6)]) tell us that:

$$\langle \sigma_i \sigma_l \rangle = \langle \mathrm{th}(\beta \Sigma_k J_{ik} \sigma_k) \, \mathrm{th}(\beta \Sigma_j J_{lj} \sigma_j) \qquad \text{if} \quad J_{il} = 0. \tag{4}$$

Now it is quite evident that for not too large β the r. h. s. fluctuates much less that the l. h. s.

This technique may be applied to the study of the expectation value of the thermal Wilson loop with a gain in computer time which may be very high $(O(10^2))$[(7)]. Similar DLR equations can also be used to decrease the statistical errors in different simulations, e. g. in the evaluation of the average value of the induced currents in the vacuum in the pseudofermions approach to fermions loops.

Let us now estimate the errors on the hadronic masses(4, 8).

In the quenched approximation for QCD the meson propagator is(1)

$$G_\Gamma(t) = \int d^3x G\ (\vec{x}, t) \propto \langle O_\Gamma(0) O_\Gamma(t) \rangle, \qquad O_\Gamma(t) = \int d^3x (\bar{q}\Gamma q)(\vec{x}, t),$$
$$G_\Gamma(\vec{x}, t) = \int d\mu[A]\ \mathrm{Tr}\left[\Gamma G_a(\vec{0}, 0; \vec{x}, t | A)\, \Gamma \gamma_5\, G_q^*(\vec{0}, 0; \vec{x}, t | A)\, \gamma_5\right] \tag{5}$$

where $d\mu[A]$ is the probability measure of pure gauge theory for the gauge field A, $G_q(\ldots | A)$ is the quark propagator in the background field A and Γ is a generic γ matrix. For the time being we suppose that we stay in a box of size L in three dimensions and infinite in the fourth direction (which we call time).

The energy of the low lying states is connected to the behaviour of $G_\Gamma(t)$ at large t, so that the dangerous errors are those which grows with t. Let us concentrate our attention on this region.

For large t wa have(4):

$$G_\Gamma(t) \equiv \int d\mu[A]\, G_\Gamma(t | A) \equiv \langle G_\Gamma(t|A) \rangle \sim \exp(-E_\Gamma t)$$
$$G_\Gamma^{(2)}(t) \equiv \langle G_\Gamma^2(t|A) \rangle \sim \exp(-E_{2\Gamma} t) \tag{6}$$

where E_Γ and $E_{2\Gamma}$ are respectively the energy of the lowest state created from the vacuum by the action of O_Γ and $O_{2\Gamma}$ where in the second case it is understood that the two quarks and two antiquarks field have different flavours (quarks interchange and quarks annihilation diagrams are forbidden).

There are two scenarios in the infinite volume limit: a) $E_{2\Gamma} < 2E_\Gamma$ because of the existence of bound states or of a continuum whose energy is smaller than $2E_\Gamma$, b) $E_{2\Gamma} = 2E_\Gamma$.

In the last case the analogy with first order perturbation theory suggest that:

$$E_{2\Gamma} \xrightarrow[L \to \infty]{} 2E_\Gamma + C \frac{l_{ZV}}{L^3 E_\Gamma} \tag{7}$$

C being a constant and l_{ZV} being the Zweig violating scattering length.

In order to understand the meaning of this result let us see what should happen in the real world by considering the cases of the pion, the rho and the delta. Generally speaking the fact that fluctuations come from Zweig violating diagrams suggest that the statistical errors are relatively small: they go to zero in the SU(n) gauge theory when n goes to infinity.

In the pion case, PCAC tell us that the pion is a quasi Goldstone boson whose scattering length should go to zero, when m_π goes to zero, as m_π^2. The fluctuations in $E_\pi \sim m_\pi$ must become proportional to $1/L^3 m_\pi$ when m_π goes to zero; note however that this result may be not true on the lattice when chiral symmetry is broken explicitely.

In the rho and delta cases let us assume that there are no exotic four quark bound states. In this situation the only danger may come from the continuum below: two pions for the rho, two pions or two rhos for the delta. Similar arguments suggest that:

$$\langle G_\varrho^2 \rangle \sim \langle G_\varrho \rangle^2 + \frac{A_{\varrho\pi}}{L^3} \langle G_\pi^2 \rangle ,$$
$$\langle G_\delta^2 \rangle \sim \langle G_\delta \rangle^2 + \frac{A_{\delta\pi}}{L^3} \langle G_\pi^2 \rangle + \frac{A_{\delta\varrho}}{L^3} \langle G_\varrho^2 \rangle^2 \qquad (8)$$

where the A's are some kind of scattering amplitudes. It is evident that in this case the fluctuations will become very large at large t: the only relief is that the prefactor of the most dangerous term ($\langle G_\pi^2 \rangle$) should become small with the pion mass.

It is now clear that a careful analysis of the statistical errors gives important informations on the Zweig violating scattering amplitudes: a full computation of the scattering length in exotic S channel states (like $\pi^+\pi^+$, pp, K^+p, ...) should not present serious difficulties, because in this case only quark interchange diagrams are present (quarks annihilation diagrams are absent).

For practical purposes it is interesting to note that the final estimate of the error on the meson propagators is essentially:

$$A/(NL^3)^{1/2} \exp(B t) \qquad (9)$$

where the prefactor should be rather small. Eq. (9) tell us that the statistical error is controlled by NL^3: in a regime where only CPU time matters and not memory, the same amount of computer time would be needed on a small and on a large lattice, the second solution being clearly the best because it minimizes the finite volume systematical effects. It is also evident that unless the amount of CPU time is really large the data at too large value of t will contain too much noise and would be useless. It would be much better to extract masses working at a very small value of t; unfortunately systematic effects are present in this region as we will see in (4).

If we restrict to the study of masses in the pure gauge sector (i. e. glueballs) the situation is strongly dependent on the method used.

The conventional measurement of correlations is very painfull and requires a too large amount of time[9]. Masses can be also extracted by considering not the correlation function but the response function, as it was pointed out in ref. (10). In these two cases the analysis of the statistical errors is straightforward and no interesting phenomena are present. The most promissing method seem to be the measurement of the linear response function by studying the difference in the signal in two different runs where the same set of random numbers has been used[10, 11]; this method does not work if the computer simulation is done using the Monte Carlo method, it works reasonably well for a Langevin type simulation[12]. Unfortunately a carefull analysis of the physical meaning and of the origine of the systematic effects in this case have not been done at the present moment.

3. - FINITE LATTICE SPACING

In computer simulations a mesh must be introduced in the Euclidean space time. It is usual to work with an hypercubic lattice, the lattice spacing being denoted by a. In an asympotically free theory without mass parameter like QCD with only zero mass quarks, only dimensionless quantities are relevant and all masses may be measured in units of a parameter Λ, which can be extracted from the experimental data on the scaling violations at high energy (in physical units Λ should stay in the range 70-200 MeV); while no parameter exists in the continuum, on the lattice we can change the value of the bare coupling constant $g_B^2 \sim 1/\beta$.

The dimensionless quantity $a\Lambda$ is a function of β, which in the relevant region of large β becomes:

$$a\Lambda = \pi(\beta)^{\omega} \exp\left[-\beta C_1 + C_o + C_1/\beta + ...\right] \qquad (10)$$

where the constants ω and C_1 can be computed in the continuum while a computation on the lattice is needed to obtain C_o. The presence of corrections proportional to high powers of β^{-1} is rather annoying: a safe estimate would consider that $a\Lambda$ is known in the relevant region inside a factor two of uncertitude until the next order correction has will be computed; at the present moment it is rather useless to compare the value of Λ extracted from different forms of the lattice action.

The situation changes if we consider quantities which have a direct physical meaning, e.g. the ratio $R(\beta)$ of the masses of two glueballs with different quantum numbers. Here for large β we have that:

$$R(\beta) = R(\infty) + O(a^2\Lambda^2) = R(\infty) + O(\exp(-C_1\beta)) . \qquad (11)$$

The corrections to the continuum result are exponentially small in β. Better results can be obtained if, as stressed by Symanzik[12], we start to change the form of the lattice action; roughly speaking we have:

$$R(\beta) = R(\infty) + a^2\Lambda^2(s_o + s_1/\beta + s_2/\beta^2 + \ldots\ldots) . \tag{12}$$

The quantities s_k depend on the lattice action, there is a form of the action such that all the $s_k^!$ are zero; moreover it is possible by a K loop computation on the lattice to extract the form of the action for which all the s_k for $k < K$ are zero.

It is therefore possible to find a form of the lattice action such that the effects of finite lattice spacing should be very small; Monte Carlo experiments for the O(3) two dimensional sigma model[14] and analytic results for the $O(\infty)$ model[15] show that a definite improvement is obtained also if one consider only a simple form of the action in which only three diagrams have been used to find the coefficients of the lattice action.

It is reasonable to think that after the improvement of the action the spectrum of the low lying states will be slightly modified for a lattice spacing of 0.1 F (and may be 0.2F) with respect to the continuum values.

4. - FINITE TIME

We have seen in (2) that the statistical errors in the propagator increase exponentially with the time so that it would be much better to extract the masses of the states from measurements done at small values of t. Generally speaking the comparison of Euclidean and Minkowski field theories tell us that the

$$G_A(t) = \langle A(t)A(0)\rangle = \sum_1^\infty{}_n \exp(-E_n|t|)\left|\langle 0|A|n\rangle\right|^2/E_n . \tag{13}$$

Only in the region where

$$\exp((E_2 - E_1)|t|) \gg \left|\langle 0|A|2\rangle\right|^2/\left|\langle 0|A|1\rangle\right|^2 \tag{14}$$

we can safely approximate $G_A(t)$ with $\exp(-E_1|t|)\left|\langle 0|A|1\rangle\right|^2/E_1$.

If $\left|\langle 0|A|2\rangle\right|^2/\left|\langle 0|A|1\rangle\right|^2$ would be a number of order 1 the effective mass

$$m(t) = -\frac{d}{dt}\ln\left[G_A(t)\right] \tag{15}$$

should be near to the true mass for not too large t.

Unfortunately if A is a local operator in space (it must be a local operator in time if eq. (13) is correct) in 4 dimensions it has at least dimension 3 for mesons and dimension 4 1/2 for barions and the transition matrix elements $|<0|A|n>|^2$ strongly increase with n. In other words an high dimensions operator is much more coupled to high mass states thet to low mass states. In this situation we need to study the behaviour of G_A at somewhat large t. We face an empasse: if t is small the estimated mass is not the true mass and if t is large the statistical error may be to large nothing may be measured.

As stressed by Wilson[16] the situation may be improved if we consider a set of operators A_i and we study the correlation matrix[17]

$$G_{ik}(t) = < A_i(t) A_k(0) > = \sum_{1}^{\infty}{}_n \exp(-E_n(t)) \frac{<0|A_i|n><n|A_k|0>}{E_n} \qquad (16)$$

Up to now this method has been mainly applied to the study of the glueball spectrum with only somewhat marginal effects[17] (in most of the cases the estimated mass was only slightly smaller than the one estimated in the naive approach). One of the possible reasons of this marginal improvement is the following: this method is mostly efficient if the operators A_i are really differents one from the other, so that they have different matrix elements with different states. It is quite possible that the operators used in numerical simulations where to similar (e. g. a plaquette of lattice side 1 and lattice side 2) and the method would have been much more successfully if also quite different operators (e. g. plaquettes of much higher side) would be included.

It is rather evident that the natural thing to do would be to construct block variables by averaging the gauge fields and the quark field in space and later to construct the meson and the glueball fields by using the block variables fields. Some minor problems are posed by gauge invariance: fields at different points of the space transform in a different way. This difficulty may be bypassed or by averaging after that the appropriate parallel transport has been done or by averaging operators at different points after a gauge fixing.

Although the question of the best choice of the set of operator is not a very deep question, it is related to the physical structure of the hadrons in a very straightforward way and its solution is a crucial step if we want to have a good mesurement of the hadronic spectrum beyond the π, ρ, p and Δ. Careful and systematic investigations in this direction would be highly welcome.

5. - FINITE VOLUME

Finite volume effects are very important; their study is no so straightforward especially in gauge theories and this has caused a certain amount of misunderstanding, e.g. it has been claimed that finite volume effects may be estimated in the framework of the potential theory (in this case they wouls be terrible high[18]). Fortunately enough potential theory is not a good representation for QCD and finite volume effects are much smaller than what estimated in this way.

For semplicity of arguments it may be much better to consider the case in which only one spatial direction is finite while all the other dirations are infinite; of course this is not a realistic situation, however as soon as finite volume effects are small, it may be reasonable to suppose that the total finite volume effects are the sum of those coming from each direction independently. If only one direction is finite and periodic boundary conditions have been used general arguments tell us that finite volume effects goes to zero like $\exp(-mL)$, m being the mass gap.

Let us consider in detail the case of pure gauge theories in the limit $N \to \infty$. The same analysis of ref. (19) tell us that we have two regimes: a confined phase in which the thermal loops are disorded and a deconfined phase where the average of thermal loops is different from zero. If one direction is finite (of length L), the system stays at a temperature T equal to $1/L$. In the confined low temperature phase the free energy of the system can be written as the zero temperature free energy plus a temperature dependent term which has a simple expression in terms of the spectrum and the S matrix of the system. Now when N goes to infinity, the spectrum and the S matrix have a finite limit, while the zero temperature free energy is proportional to N: the relative variation of the free energy with L disappear in the low temperature phase when N goes to infinity; this phenomenon is the translation in physical terms of the Eguchi Kawai[20] effect for pure gauge theory. Of course in the high temperature phase, where confinement does not hold anymore, the free energy will have a non trivial dependence on L.

This analysis implies that for the physical case (N finite) finite volume corrections will be rather small (i.e. proportional to $1/N$) as soon thermal and space loops are disordered. For the SU(3) case the confinement-deconfinement transition is rather sharp (firt order[21]) and happens at a temperature of about 350 MeV which corresponds to a box side of about 0.6 F[22] (the value of L at which the space and thermal loops are disordered may be slightly different in the case of only one direction finite or of 4 directions finite).

If we want to have small finite volume effects we need to stay in a situation where the loops winding through the lattice are disordered: it is therefore necessary in computer simulations with small lattice to monitor them.

The same analysis may be extended to the case where quarks are present: if we restrict ourselves to the quenched approximation we notice that also in the high temperature phase finite volume effects for fermions are depressed by the presence of the gauge fields: the existence of different gauge configurations having the same action but a value of the space loops which differs of an element of the center of the group (Z_3), implies that the momenta of the quark can take the following values:

$$P_n = \frac{2\pi}{3L} n \qquad n = 0, \ldots, 3L-1 \tag{17}$$

not $\frac{2\pi}{L}n$ has happens in the free theory without gauge fields. In other words the quarks feel a volume which is three times larger of the true one(23). This fact explains why finite volume effect cannot estimated from potential theory. Of course the hadrons are singlects of SU(3) coulor and they do not feel Z_3 transformations: finite volume effects on the masses of the hadrons can be related to the physical static potential between Hadrons: a naive estimate for large L is(1)

$$E(L) = E(\infty) + 6\ V_h(L) \tag{18}$$

where $V_h(r)$ is the static hadronic potential. A more careful analysis(8) shows that eq. (18) is essentially correct for the baryons, while for the mesons only the Zweig violating part of the potential is relevant. The experimental fact that strong forces between quarks are essentially saturated and that the residual hadron-hadron force is relative weak (it disappear when N goes to infinity) indicates that finite volume effects should be much smaller that the estimates which can be done by assuming a non relativistic potential model for the quark-quark interaction.

At any rate it is clear that is better to work on boxes which are not too smaller than the diameter of the hadron. A naive estimate of the hadron diameter can be taken to be the square root of the cross section at intermediate energies (i. e. 10 GeV).

If we use the experimental data and the SU(3) flavour symmetry we find that the proton diameter is 1.8 F while the pion diameter is 1.2 F: if we substitute strange quarks to the light quarks the hadronic radius should go down of a factor 2.

A qualitative estimate of the finite volume effects for the proton may be obtained by considering a box such that the system has the same density of the nuclear matter: this happens for a box of about 1.8 F; in this situation we expect to have a shift in the proton energy of the order of the nuclear matter binding energy, i. e. 14 MeV.

The reader interested in planning a computer experiment may be use these informations as he like; personally I would reccomend a box of at least 0.8 F for any kind of measurement; on such a box the masses of strange hadrons may be reasonably estimated, the masses of the strange baryons likely need a larger box (1F) while the nucleon needs a larger box (1.5-2 F).

It may be sound strange that I am suggesting to use boxes just of the same size of the lighthest physical particles (i. e. the pion whose mass is about 1.5 F). Fortunately enough the pion is a quasi Goldstone boson who decouples (as we have already seen) in the zero mass limit: everything must be finite when the pion aquires zero mass also in a finite box. It is useful to remark that this last statement is true if the chiral symmetry is spontaneously broken on the lattice explicitely, the pion acquires a residual interaction which does not vanishes in the zero mass limit. At the present moment it is unclear how much this effects is really annoying: it shows up in the fluctuations of the critical value of K at which the pion becomes massless in the Wilson theory. If it is needed, drastic decision can be taken, e. g. averaging the quark propagator (not the hadronic propagator) over configurations which differs for Z_3 transformations.

6. - EXTRAPOLATION IN THE QUARK MASSES

As we have seen from the previous sections both systematic and most unfortunately statistical errors increase strongly by decreasing the quark masses (this last point has been compleately lost in the analysis of ref. (24)). This difficulty may be bypassed by studying theories where the up and down quarks have a mass high than the physical one, only at the end extrapolate at nearly zero mass. This procedure is imperative for the lattices of the present dimensions and it is likely that the computation of the hadronic masses at the physical point (i. e. pion mass equal to 140 MeV) will be an useless and time consuming effort also in the near future. Indeed quantities like the width of the ρ or the Δ, which are very sensitive to the pion mass, cannot be compute directly (they can be estimated from the knowledge of the $\rho\pi\pi$ or $\Delta p\pi$ couplings which can be obtained or from vector meson dominance or PCAC) while other quantities are reasonable smooth functions of the quark mass.

It is a general rule that reasonable extrapolations are possible only if something is known on the function we need to extrapolate; in the present case the dependence of physical quantities on the quark masses has been widely studied in the contest of chiral perturbation theory[25]: no analytic terms like $m_q^{3/2}$ or $m_q^2 \ln m_q$ (m_q being the quark mass) are present whose coefficients are known as function of the chiral parameters (e.g. f_π or g_A). It is quite reasonable (also if we consider the success of the Gellman Okubo sum rule), that a careful computation of the hadronic spectrum and of the low energy coupling constants in the region where the pion mass is not smaller that 300--400 MeV will be more than enough to obtain quite reliable extrapolations if the results of chiral perturbation theory are used.

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