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Talk given at the Trieste Meeting,
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THEORETICAL ASPECTS OF COMPUTER EVALUATIONS OF THE HADRONIC MASS SPECTRUM

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In these last years we have seen computations of the hadronic mass spectrum[1,2]; now, due to the relatively small size of the lattice (which ranged from $5^3 \times 10$ to $8^3 \times 16$) these evaluations are affected by uncontrolled systematical errors: the lattice spacing is not small enough and the box is not too large. These computations cannot be used at the moment for a sound verification of QCD but open the road to larger scale simulations for which the systematical errors will be under control.

Although the standard Monte Carlo technique is an ingredient of most (but not all) of these works, the evaluation of the mass spectrum cannot be done by using a naive approach: there are many theoretical problems which must be solved to reach such a goal. In this talk I will concentrate on some of them (mainly those which I have directly studied, because I know them better). I would like to convince the audience that in this field there is a lot of work that can be done in the usual way that theoretical physicists are accustomed to: with paper and pencil.

To introduce the subject let me tell you how happened that I started to be interested in these kind of problems. When Wilson firstly[3] discussed the feasibility of large scale Monte Carlo simulations for gauge theories to extract the renormalization group trajectories for the effective Hamiltonian of the block spin variables, the most natural question was why not to compute directly the mass spectrum instead of the effective Hamiltonian. Well, my naive answer at this question at that time was that a computer evaluation of the mass spectrum was impossible: let me explain why I had such an opinion and how the difficulties have been later removed.

We consider for time being a theory with only Bose fields in a box of size $L^3 \times T$. The vacuum expectation value of a functional $g[\varphi]$ of the field φ in the Euclidean theory can be written, as stressed by Symanzik long time ago, as a statistical expectation value:

$$\langle g[\varphi] \rangle = \int d\mu[\varphi]\, g[\varphi], \quad d_\mu[\varphi] \propto d[\varphi] \exp\left[-S[\varphi]\right] \tag{1}$$

$$\int d\mu[\varphi] = 1$$

where $d\mu[\varphi]$ is a probability measure and $S[\varphi]$ is the Euclidean action.

If the operator $O[\varphi]$ acting on the vacuum creates a single particle state of mass m plus other stuff at higher mass, we know that:

$$G_o(n) = \langle O(n)\, O(0) \rangle \sim \frac{|\langle 0|O|m\rangle|^2}{2m} \exp(-mna) \tag{2}$$

$$O(n) = \sum_{\vec{\tau}} O(\vec{\tau}, n) \qquad 0 \ll na \ll T/2a$$

where $\vec{\tau}$ and n denotes the coordinates in the space and time directions respectively, a being the lattice spacing. The mass m depends obviously on L but if there is a mass gap m(L) differs from m(0 0) by terms which are exponentially small in L for large L.

An elementary evaluation tell us that the naive idea of computing the correlation function by Monte Carlo (i. e. by constructing N equilibrium configurations and by measuring the correlation function in the interesting region by direct averaging of the operator O in the interesting region) cannot work for small lattice spacing in a 4 dimensional gauge theory. Indeed equation (2) is valid only if the euclidean time (t + na) is much larger than the inverse of the gap between the one particle state and the first excited state (and still much smaller than a T/2). We have to see a signal in the region where it is exponentially small and measure the slope of the signal: if the algorithm is deterministic, we are bounded only by the rounding error of the computer; unfortunately the

Monte Carlo method is of probabilistic nature: after N iterations we have that

$$(G_o(n))_M = G_o(n) + r\left[G_o(0)/N\right]^{1/2} \tag{3}$$

where $(G_o(n))_M$ is the measured correlation and r is a random distributed number with unit variance.

The independence of the noise on the distance makes particularly hard to measure the signal at large distances where it is exponentially small: this problem may be partially alleviated by taking N quite large (e.g. 10^6); the real difficulty which is going to kill the naive approach is that of 0 is an operator of dimension 4, G(0) is divergent, when a goes to zero, as a^{-5}: a decrease of a factor 2 in a need an increase of N of a factor 2^{10} to compensate the effects in the statistical errors. If we add that the number of points has increased of a factor 2^4 and that the Monte Carlo method is less efficient for generate independent configurations (this effect is called critical slowing down and it is likely to cost an extra factor 2^2, we finally arrive to the conclusion that the same computation with a smaller than a factor two in the scaling region will cost about 2^{16} more computer time.

In other words we have to see a cross over between the perturbative t^{-5} behaviour and an exponentially decreasing behaviour: this must be done by measuring the correlation function in regions it takes quite different values and that is practically impossible in presence of a noise which does not depend on the distance. Of course it is possible to do in reasonable time a computation with a large lattice spacing, but this strongly limits our possibilities of testing QCD in the continuum limit.

Having exposed the problem let me tell you now some of the solutions which have been found up to now, hoping that something better will be found in the future.

The first remark is that we can use the linear responce theory to partially alleviate the problem[4, 5, 6]: we suppose to add to the action a term proportional to $\varepsilon O(0)$:

$$S_\varepsilon = S - \varepsilon O(0) \tag{4}$$

and we consider the ε dependent expectation value:

$$\varepsilon R(n) = \langle O(n)\rangle_\varepsilon - \langle O(x)\rangle\Big|_{\varepsilon=0} = \langle O(n)\rangle_\varepsilon - \lim_{n\to\infty}\langle O(x)\rangle_\varepsilon = \sum_k \frac{\varepsilon^k}{k!}\langle O(0)^k O(n)\rangle_\varepsilon \tag{5}$$

While for ε small only the first term is dominant, if O^k does not excite from the vacuum particles of mass smaller than m, we have that for any value of ε the response function goes like

$$R(n) \sim \exp(-m n a). \tag{6}$$

The natural statistical error in measuring the responce function is:

$$(O(0)/L^3N)^{1/2}, \tag{7}$$

while also if we consider

$$\frac{1}{T} \sum_{1}^{T}{}_m \langle O(m)\, O(n+m) \rangle,$$

the error for the correlation function is:

$$(O(0)/TN)^{1/2} \sim (O(0)/LN)^{1/2}, \tag{8}$$

(we assume that T is of order L, as happens in most of the cases).

By comparing eq. (6) and (8) we see that we have gained a factor L in the statistical error, which corresponds to a factor L^2 in computer time. If L = 10 this is a gain of a factor 100, which although not negligeable, is not the solution to our problems. What really need in an algorithm which has an intrinsic error which exponentially decrease with the distance. This can be done if we can in some sense cancell the effects of the randomness of the Monte Carlo approach.

The first suggestion would be to do two Monte Carlo simulations, one at $\varepsilon = 0$, the other at small ε (e. g. $\varepsilon = 10^{-2}$) using in the two simulation the same sequence of random numbers and to evaluate directly:

$$R(n) = \frac{1}{\varepsilon}\left[\langle O(n) \rangle_{\varepsilon} - \langle O(n) \rangle_{\varepsilon_0}\right] \tag{9}$$

hoping that the fluctuations are the same in the two cases, so we should see the signal directly. However due to the nature of the Monte Carlo method, the difference between the two configurations (with action S_ε and $S_{\varepsilon=0}$ respectively) will be or 0 or 0(1) but cannot be of order ε. This difficulty can be solved if we use an algorithm whose output depends in a differentiable way on the action S (the output of the Monte Carlo is not continuous in S). An example of this algorithm is provided by the Langevin equation[7], which we write for semplicity in the case of a scalar ϕ^4 field theory:

$$\dot{\phi} = (-\Delta + m^2)\phi + g\phi^3 + \eta = -\frac{\delta S}{\delta \phi} + \eta \tag{10}$$

where η is a Gaussian distributed with noise with covariance:

$$\overline{\eta(x,t)\,\eta(x',t')} = 2\delta(x-x')\delta(t-t'). \tag{11}$$

It is well known from the beginning of this century that the time average[F1] of a solution of eq. (10) with a given realization of the noise gives the normal statistical expectation value. In this way the Langevin equation for continuous variables is a visible alternative to the Monte Carlo.

We can now use an ε dependent action in eq. (10), compute two trajectories for different values of ε and use the eq. (9) for evaluating the response function in the limit $\varepsilon \to 0$.

If $g = 0$ the algorithm is no more probabilistic, but becomes deterministic when $0 = \varphi$:

$$\dot{\varphi} = -(-\Delta + m^2)\varphi + g\varphi^3 + \eta \ , \qquad \dot{R} = -(-\Delta + m^2)R + 3g\varphi^2 R \cdot \delta(x) \ , \tag{12}$$

$$R(x) = \lim_{\tau \to \infty} \frac{1}{t} \int_0^t R(x,t')\,dt' .$$

If g is different from zero the algorithm is probabilistic, but one can prove at all orders in perturbation theory that the error on R is exponentially small when the distance becomes large. However the algorithm must be used in a region where perturbation theory does not converge too well so that it is usefull to see what happens in different cases.

On a linear chain for $m = 0$ and $g = 1$ the algorithm is perfect[4]: correlations function may be evaluated also in regions where there are of order 10^{-20} without dificulties, implying a gain in computer time of 10^{40}. In more realistic models like the non linear sigma model in two dimensions I have observed[4] a gain factor of order 10^{16} for the O(N) model (N 4) while a gain of only 100 was observed for O(3): the reason for this drastic difference are not clear.

The algorithm has been implemented for measuring the glueball mass in 4 dimensional SU(2) gauge theory[2], where an improvement factor of order 10^{3-4} have been observed (given the two dimensional experience we may hope that something better can be done for SU(3)).

Methods based on the Langevin equation seem to be the most promising one for accurate determination of the glueball mass spectrum. Let us now see how these ideas can be extended to Fermions. The key point that we need to implement is that although some probabilistic method must be used, the computation of the correlation must be done as far as possible using deterministic algorithms. We consider now the case of QCD in the continuum and we do not address to the problems connected with lattice regolarization. If the euclidean action is written as:

$$S = \Sigma_f \psi_f (\not{\partial} + m)\psi_f + S(A) \tag{13}$$

the gauge fields have the following probability measure:

$$d\mu[A] \propto d[A]\,[\det(\not{\partial} + m)]^{n_f} \exp[S(A)] \tag{14}$$

n_f being the number of quark flavours (for semplicity of equal mass).

We pospone the problem of finding the algorithm to extract the gauge fields with such a probability distribution and we concentrate on the evaluation of the masses of particles having internal flavour quantum numbers different from zero. For a given gauge field configuration, the quark propagator can be computed using the same approach as before (eq. (12)), the action being quadratical in the quark fields:

$$\langle \bar{\psi}(x)\psi(0)\rangle_A = G^q(x|A) = \lim_{t\to\infty} G_t(x|A) \tag{15}$$

where $G_t^q(x|A)$ satisfies the deterministic equation[8]:

$$G_t^q(x|A) = -(\not{\partial} + m)G_t^q(x,A) + \delta x\,. \tag{16}$$

The pion propagator can be written as

$$G_\pi(x) = \int |G^q(x|A)|^2\, d\mu[A] \tag{17}$$

where we have neglected flavour dependent factors; similar formulae hold for different propagator.

The strategy is now clear: we extract the gauge field configuration with their probability distribution, we evaluate the quark propagator with a deterministic algorithm and we use the quark propagator to compute the hadronic correlation functions.

We should now evaluate the statistical errors induced by this procedure. This can be done if we know the expectation value of $|G^q(x)|^4 = G_{\pi\pi}(x)$, the relative error on G_π being given by:

$$(G_\pi(n))_{\text{measured}} = G_\pi(n) + r\,G_{\pi\pi}(n)/N)^{1/2}\,. \tag{18}$$

An elementary computation[9] shows that if L is large and if no pion pion bound states are present:

$$G_{\pi\pi}(n) \sim \exp\left[-\frac{\alpha |m_\pi^{-1}}{L^3}\, na\right]\left[G_\pi(n)\right]^2 \tag{19}$$

where α is the pion pion scattering length (which must be negative) arising from Zweig violating diagrams, which from fenomenological considerations is supposed to be quite small on the normal hadronic scale.

We easily see that although the relative error is slowly increasing with t, the absolute error is practically of the same order of the correction itself, moreover if t goes to infinity together with L, the error in extimating the correlation (and the mass) of the pion decrease like $1/L$ $(1/L^2)$, so that only one quark propagator would be enough in the infinite volume limit to obtain the mass of the pion: the most likely mass coincide with the true mass. The same result hold for the proton, while a mere careful analysis must be done for the other particles.

The situation is quite satisfactory, as far statistical errors are of the order of magnitude of the signal itself so the can easily reduced without a too large increase in the number of configurations to be considered. If we implement this program by setting $n_f = 0$ in the probability measure for the gauge fields, we obtain the so called quenched approximation[8]; in this case we can extract the gauge field configurations using the standard Monte Carlo technique and the vacuum polarization diagrams of the quarks are neglected[10].

In the realistic situation $n_f \neq 0$ and the direct evaluation of the determinant is so painfull that the Monte Carlo method can be applied only on very small lattice. A practical algorithm for extracting the gauge fields configurations with the correct wheight have been proposed in ref. (11); we present it in the case of the Langevin equation[12] (we can find an equivalent version for Monte Carlo). We consider the following coupled differential equations:

$$\begin{aligned} \dot{A}_\mu &= -\frac{\partial S}{\partial A} - n\phi\,\gamma_\mu \not{\partial}\,\phi + \eta_A \\ \dot{\phi} &= -(\not{\partial} + m)(-\not{\partial} + m)\,\phi/\tau + \eta_\phi/\tau^{1/2} \end{aligned} \tag{20}$$

where the η's are as usual white noises.

If $n = 1$ the time average of the solution of eq. (20) are the statistical expectation values evaluated with the action:

$$S(\phi, A) = S(A) + \phi(-(\not{\partial})^2 + m^2)\,\phi \tag{21}$$

where ϕ is a normal spin 1/2 Boson. This results holds independently of τ and can be proved order by order in perturbation theory[7]. If we set $n = -1/2$ and we send τ to zero, we can argue that the A_μ fields are distributed according to eq. (14), with an error of order a; a direct digramatical proof of this fact in perturbation theory is available[12].

I have sketched how to generate the gauge fields configurations to be used for the evaluation of non flavour singlest hadrons; the computation for hadronic singlests can be done by measuring the appropriate response function, as discussed in ref. (9).

I have outlined here the strategy that should lead to a verification (or to a falsification) of QCD as far the hadronic mass spectrum is concerned. This strategy may be not the best one, but it is the only one available at the present moment. Also if we do not try to change strategy there is still much theoretical work to be done, among the various open problems let me quote the search of the best efficient method for computing the quark propagator on the lattice(F2), and the completion of Symanzik's improvent program.

FOOTNOTES

(F1) - The time here is a five dimensional time (computer's time) which quite different for the four dimensional Euclidean time.

(F2) - At the present moment the quark propagator on the lattice is computed for Wilson's fermions using the Gauss Seidel method(13), but it is possible that other methods, like the coniugate gradient method of ref. (14) may be more powerful.

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