Nuclear Physics B225 [FS9] (1983) 475–496

CONSIDERATIONS ON NUMERICAL ANALYSIS OF QCD

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Received 13 June 1983

We discuss the strategy to remove the quenched approximation and to minimize systematical and statistical errors occurring in the numerical simulation of lattice QCD.

We suggest a way to compute the flavour singlet sector of the mass spectrum, and comment about the relation between the fluctuations of the mass values and the scattering amplitudes.

1. Introduction

Recently many efforts have been devoted to the analysis of the low-energy part of the hadronic spectrum and of the pattern of chiral symmetry breaking in lattice QCD. While most of the numerical work has been done using the so-called quenched approximation [9, 2–7] (i.e. neglecting the quark vacuum polarization diagrams), some recent results have been obtained for the full theory [1]. Although the results of these computations are affected by systematical errors (due for example to the small size of the lattice [8]) that are very difficult to control, they suggest (and make somehow concrete) the possibility of more precise investigations, to be done on larger lattices, which would determine the hadronic mass spectrum in a picture where systematic errors are under control and statistical errors are reasonably small.

In this paper we discuss the strategy to remove the quenched approximation. The claim that these computations can be performed by using an amount of CPU time comparable with the time needed for a quenched computation is supported by the results of the numerical simulations [1] we mentioned above.

In sect. 2 we review the general formalism [9–11, 2–4] for numerical simulations of lattice gauge theories with fermions. In sect. 3 we study the sources of systematic errors affecting the evaluation of the effects of quark loops, and we suggest the

computational methods to be preferred. In sect. 4 we outline how the computation can be organized.

Three appendices focus on specific problems: in appendix A we show how to compute the flavour singlet ($I=0$) sector of the mass spectrum. In appendix B we discuss the relation between the fluctuation of the mass values and the scattering amplitudes, and about the formation of many quark bound states. In appendix C we give some details about our computer codes, and we suggest efficient computational methods.

2. Dealing with fermionic theories: the general formalism

2.1. THE LATTICE FERMIONIC THEORY: EFFECTIVE ACTION AND SECOND-ORDER FORMALISM

Let us consider a lattice theory, characterized by the following euclidean action:

$$S[A,\bar{\psi},\psi]=S_{\mathrm{G}}[A]+\sum_{f=1}^{n_{\mathrm{f}}}\bar{\psi}_i^{(\mathrm{f})}\Delta_{ik}[A]\psi_k^{(\mathrm{f})}\,, \tag{2.1}$$

where A stands for the set of bosonic fields defined on the links of the lattice, ψ for the set of fermionic fields defined on sites, i and k denote the lattice sites, n_{f} is the number of flavours. Although the action of eq. (2.1) has a quite general form, in the following discussion we will assume that the A fields are gauge fields and that the ψ fields are quarks.

Using the Matthews–Salam formula [12] we can rewrite the mesonic and the baryonic propagator in the following way (for the sake of simplicity we will drop color, flavour and spinor indices):

$$\langle\bar{\psi}(x)\psi(x)\bar{\psi}(0)\psi(0)\rangle_{I\neq 0}=\int \mathrm{d}\mu_{\mathrm{eff}}[A]\,\Delta^{-1}_{x,0}[A]\Delta^{-1}_{0,x}[A]\,, \tag{2.2a}$$

$$\langle\bar{\psi}(x)\psi(x)\bar{\psi}(0)\psi(0)\rangle_{I=0}=\int \mathrm{d}\mu_{\mathrm{eff}}[A]\,\Delta^{-1}_{x,0}[A]\Delta^{-1}_{0,x}[A] - n_{\mathrm{f}}\int \mathrm{d}\mu_{\mathrm{eff}}[A]\,\Delta^{-1}_{0,0}[A]\Delta^{-1}_{x,x}[A]\,, \tag{2.2b}$$

$$\langle\bar{\psi}(x)\bar{\psi}(x)\bar{\psi}(x)\psi(0)\psi(0)\psi(0)\rangle=\int \mathrm{d}\mu_{\mathrm{eff}}[A]\,(\Delta^{-1}_{x,0}[A])^3\,, \tag{2.2c}$$

where

$$\begin{aligned}\mathrm{d}\mu_{\mathrm{eff}}[A]\propto \mathrm{d}[A]\,\mathrm{e}^{-S_{\mathrm{eff}}[A]}&=\mathrm{d}[A]\,\mathrm{e}^{-S_{\mathrm{G}}[A]}\det{}^{n_{\mathrm{f}}}\Delta[A]\\&=\mathrm{d}[A]\exp\{-[S_{\mathrm{G}}[A]-n_{\mathrm{f}}\,\mathrm{Tr}\,(\ln\Delta[A])]\}\,,\\ \int \mathrm{d}\mu_{\mathrm{eff}}[A]&=1\,.\end{aligned} \tag{2.3}$$

By $I=0$ we denote the flavour singlet sector; we will assume that flavour symmetry is unbroken.

Fermions on the lattice are usually described by the Wilson [13] or the Kogut–Susskind [14–16] (KS) formalism: in both schemes the determinant of Δ is a real number, and it is positive in the KS picture. In both cases the operator Δ is not hermitian; however we can use the following relation*

$$\det(\Delta)\in\mathbb{R}^+\Rightarrow\det(\Delta)=[\det(\Delta)\det(\Delta^*)]^{1/2}$$
$$\Rightarrow\det(\Delta)=\det(\Delta\Delta^*)^{1/2}\equiv\det(\tilde{\Delta})^{1/2},$$

in order to deal with a hermitian operator. Substituting $\tilde{\Delta}$ for Δ in (2.3) yields a theory with $2n_f$ flavours; for the continuum this procedure corresponds to the use of a second-order formalism theory [17, 9], i.e. to quantize the action

$$\bar{\psi}(-D_\mu D^\mu+\sigma_{\mu\nu}F^{\mu\nu}+m^2)\psi,$$

where the ψ are parafermions of order $\frac{1}{2}$. Substituting at the same time $\tilde{\Delta}$ for Δ and $\frac{1}{2}n_f$ to n_f we will get a theory with the same number of flavours as the original one. Now for KS fermions $d\mu_{\text{eff}}[A]$ can be thought as a probability measure; the same holds for Wilson fermions if one is in conditions such to avoid a change in sign of $\det(\Delta)$, or restricts oneself to even n_f.

The computational procedure we have in mind is the following: by using some probabilistic algorithm we produce configurations of the gauge fields thermalised with respect to the measure $d\mu_{\text{eff}}[A]$, and then we measure expectation values such as those considered in equations (2.2). The inverse operators needed for this last step (fermionic Green function) Δ^{-1}_{ik} can be obtained, with the required high precision, for the given configuration of the gauge fields by using a fast algorithm, suitable to invert sparse matrices (relaxation, Gauss–Seidel, conjugate gradient). A difficult goal to achieve is to measure the mass differences between $I=0$ and $I\neq 0$ states; we will comment about this point in appendix A.

It should be noticed that in eq. (2.3) n_f is not necessarily an integer number. This observation can be used to compensate for the species doubling of the KS fermions. The KS action gives rise, in the continuum limit, to

$$n_f^{(\mathrm{KS})}=2^{d/2}$$

fermionic species (d is the number of space-time dimensions), and setting the parameter n_f contained in the effective action to be equal to (wanted number of species)/$n_f^{(\mathrm{KS})}$ we will get the quark-loop corrections for the wanted number of flavours.

* We denote by A^* the adjoint of the operator A (hermitian conjugation)

$$(A^*)_{ik}=\mathrm{Re}\,(A_{ki})-i\,\mathrm{Im}\,(A_{ki}).$$

2.2. GENERATING THE GAUGE FIELD CONFIGURATIONS

We discuss now the algorithm which can be used to generate configurations of the gauge fields A with the measure $d\mu_{\rm eff}[A]$. We will temporarily forget the unitarity constraint on A. These will be considered in sect. 4.

Let us outline two possible computational methods. The first possibility consists in writing an equation "à la Langevin" for the fields $A_i(t)$ (t is in this case the Langevin time):

$$\begin{aligned}\frac{dA_i}{dt} &= -\frac{\delta}{\delta A_i}(S_{\rm eff}) + \eta_i(t) \\ &= -\frac{\delta}{\delta A_i}(S_{\rm G}) + n_{\rm f}\,{\rm Tr}\left\{\Delta^{-1}\frac{\delta}{\delta A_i}(\Delta)\right\} + \eta_i(t) \\ &= -\frac{\delta}{\delta A_i}(S_{\rm G}) + \tfrac{1}{2}n_{\rm f}\,{\rm Tr}\left\{\tilde{\Delta}^{-1}\frac{\delta}{\delta A_i}(\tilde{\Delta})\right\} + \eta_i(t)\,, \end{aligned} \tag{2.4}$$

where $\tilde{\Delta} = \Delta\Delta^*$, and $\eta_i(t)$ is a gaussian white noise with

$$\overline{\eta_i(t)\eta_j(t')} = 2\delta_{ij}\delta(t-t')\,. \tag{2.5}$$

The other possibility would be to use the Metropolis algorithm [18]. One A field at once is updated each time: the new tentative field $A_i^{\rm T}$ is given by

$$A_i^{\rm T} = A_i^0 + \rho r_i\,, \tag{2.6}$$

where A_i^0 is the old value of the field, r_i is a random 3×3 matrix, with elements such that

$$\langle r_i^{ab}\rangle = 0\,, \qquad \langle |r_i^{ab}|^2\rangle = 1\,,$$

($a, b = 1, 2, 3$), and ρ is a control parameter. We should remind the reader that in this analysis we are neglecting the constraint $A_i \in {\rm SU}(3)$, that is implemented in the actual computation. Now we will select the new value for our field A_i (we call $A_i^{\rm N}$) by setting $A_i^{\rm N} = A_i^{\rm T}$ with probability p (exchange is performed) and $A^{\rm N} = A^0$ with probability $(1-p)$ (no change). The probability p is given by

$$\begin{aligned} p &= \min\{\exp\{-(S_{\rm eff}[A^{\rm T}] - S_{\rm eff}[A^0])\}, 1\} \\ &\equiv \min\{p_{\rm T}, 1\}\,. \end{aligned} \tag{2.7}$$

For small ρ we can write

$$\begin{aligned} p_{\rm T} &= \exp\left\{-\frac{\delta S_{\rm eff}}{\delta A_i}\rho r_i + {\rm O}(\rho^2)\right\} \\ &= \exp\left\{-\left[(S_{\rm G}[A_{\rm T}] - S_{\rm G}[A_0]) - \tfrac{1}{2}n_{\rm f}\rho r_i\,{\rm Tr}\left\{\tilde{\Delta}^{-1}\frac{\delta}{\delta A_i}\tilde{\Delta}\right\}\right]\right\}, \end{aligned} \tag{2.8}$$

where terms of order ρ^2 are neglected. Here ρ is a free parameter, that we can choose small enough for $O(\rho^2)$ in (2.8) to be negligible; we will have to however pay the price in the time of approach to equilibrium which grows as ρ^{-2}.

The two methods we have proposed can be related through a Kolmogorov result [19]: if we identify

$$t = \rho^2 n ,$$

n being the number of times we upgrade "à la Metropolis" each of our link variables, in the limit where ρ goes to zero at fixed time t the Kolmogorov equation for the evolution of the transition probability for the A fields will tend to the Fokker–Planck equation associated to the Langevin eq. (2.4). In simpler words a Monte Carlo simulation with small up-dates is equivalent to a Langevin equation. The Monte Carlo procedure for continuous variables can be considered as a wise (the asymptotic equilibrium distribution is preserved) discretization in time (introducing a mesh for the time variable) of the Langevin equation.

It seems to us that, if the lattice size is not too small to get sensible physical results, the only possibility of avoiding the need of enormous computer time and/or of an unacceptably large quantity of computer memory lies in performing small average up-dates of the gauge fields, independently of the upgrading method chosen.

Using p_T as in eq. (2.8) for a non-zero ρ we expect to find an error of order ρ on the equilibrium distribution $d\mu_{\text{eff}}[A]$.

The limit $\rho \to 0$ can be taken in different ways: we can compute the physical quantities we are interested in for a few different small values of ρ, and extrapolating the result to $\rho = 0$ (after verifying that we are in a zone in which a linear extrapolation makes sense). The other possibility is setting ρ to such a small value $\tilde{\rho}$ that $\langle 0 \rangle_{\rho=\tilde{\rho}} - \langle 0 \rangle_{\rho=0}$ is negligible. To this respect we want to remark that the contribution to the RHS of eqs. (2.4) and (2.8) due to the fermion fields should in principle be updated every time that a single link variable is substituted. In the $\rho \to 0$ limit updating this contribution, for example, just after one full sweep on all the gauge fields A, will induce on the equilibrium probability an error vanishing with ρ.

2.3. THE FERMIONIC CONTRIBUTION TO THE ACTION

We come now to the crucial point: how to compute $\mathrm{Tr}\{\tilde{\Delta}^{-1}(\delta/\delta A)\tilde{\Delta}\}$, appearing in (2.4) and (2.8). The computation of $((\delta/\delta A)\tilde{\Delta})_{ik}$ is straightforward: using the lattice equivalent of the second-order formalism only elements for which i and k are at most second-nearest-neighbour sites will be non-zero. So we are left with the computation of the elements of $(\tilde{\Delta}^{-1})$. Let us analyze some efficient techniques.

The first possibility (defermionization) consists in building an auxiliary Monte Carlo procedure for some auxiliary bosonic fields φ_i (lying on sites) that we call

pseudofermions [10, 9]. We start from the identity

$$(\tilde{\Delta}^{-1})_{ik} = \int \mathrm{d}\mu[\varphi]\varphi_i^* \varphi_k ,$$

$$\int \mathrm{d}\mu[\varphi] = 1 ,$$

$$\mathrm{d}\mu[\varphi] \propto \mathrm{d}[\varphi] \exp\left\{ -\sum_{lm} \varphi_l^* \tilde{\Delta}_{lm} \varphi_m \right\}, \tag{2.9}$$

which suggests to us that we compute the two-point function of the φ field (with measure $\mathrm{d}\mu[\varphi]$) by a Monte Carlo procedure consisting of n_{PF} sweeps on all the φ fields. We can now precisely expose the full recipe for constructing a configuration of A fields in equilibrium with $\mathrm{d}\mu_{\mathrm{eff}}[A]$. Each complete cycle will consist of two phases. First one does n_{PF} Monte Carlo sweeps for the φ fields (using the probability measure of eq. (2.9)), and afterward updates once the A fields (on the whole lattice) using, in (2.4) or (2.8),

$$\mathrm{Tr}\left\{ \tilde{\Delta}^{-1} \frac{\delta}{\delta A_i} \tilde{\Delta} \right\} = (\tilde{\Delta}^{-1})_{lm} \frac{\delta}{\delta A_i} \{\tilde{\Delta}_{ml}\}$$

$$\simeq \frac{\delta}{\delta A_i} \{\tilde{\Delta}_{ml}\} \overline{\varphi_m^* \varphi_l}$$

$$= 2\,\mathrm{Re}\left[\Delta_{mk}^* \frac{\delta}{\delta A_i} \{\Delta_{kl}\} \overline{\varphi_m^* \varphi_l} \right], \tag{2.10}$$

where the bar denotes the average over the last $(n_{\mathrm{PF}} - n_{\mathrm{D}})$ iterations over the pseudofermions, where n_{D} stands for the number of iterations used at the beginning of any pseudofermionic cycle for bringing the pseudofermions to equilibrium, and not used in computing average values (discarded). The error intrinsic to this approximation vanishes in the limit $1/n_{\mathrm{PF}} \to 0$. It should be noticed that the limit of small ρ implements the limit of small $1/n_{\mathrm{PF}}$: when the dynamics of the gauge fields slows down, the relative speed of the pseudofermionic one becomes greater.

It is clear that the second-order pseudofermionic formalism we have built up can be used independently from the probabilistic algorithm we choose to update the pseudofermions: a good choice to construct the equilibrium probability $\mathrm{d}\mu[\varphi]$ may be to use the heat bath method [20]. The main reason which makes this procedure very convenient for the upgrading of pseudofermions is that the φ equilibrium probability is gaussian. Other advantages can be seen in the heat bath formulation: first there are no free parameters to be adjusted by hand (like $\overline{\delta\varphi^2}$ in the Metropolis algorithm), the procedure being optimized by itself. This is a very nice feature, because tuning parameters and trying to reach the maximum efficiency is always very demanding timewise. Secondly the heat bath is slightly faster (of a factor of order 2) than the Monte Carlo procedure, even if in the latter multiple hitting is

used [21]. Finally the computer code does not contain in this case "logical IF" statements; in other words there are no discontinuities in the evolution of the φ_i fields with respect to the variables $\Delta_{ik}[A]$. This fact will be shown to be useful when computing the splitting between $I=0$ and $I\neq 0$ masses (see appendix A).

In both methods (Metropolis and heat bath) the use of the second-order formalism is compulsory: the pseudofermion action has to contain the hermitian operator $\tilde{\Delta}=\Delta\Delta^*$. On the contrary if we want to perform a direct evaluation of $(\Delta^{-1})_{ij}$ using the first-order formalism we can consider the following set of Langevin-type equations:

$$\begin{aligned}\varphi_1^i &= -\Delta_{ij}\varphi_1^j + \eta_i(t)\,,\\ \varphi_2^i &= -(\Delta^{\mathrm{T}})_{ij}\varphi_2^j + \eta_i(t)\,,\end{aligned} \tag{2.11}$$

where

$$\overline{\eta_i(t)\eta_k(t')} = 2\delta_{ik}\delta(t-t')\,,$$

Δ^{T} is the transposed Δ and in the two equations (2.11) the stochastic noise is the same. Assuming that Δ_{ij} is a positive operator, in the sense that

$$\lim_{t\to\infty} \mathrm{e}^{-\Delta t} = 0\,,$$

we get

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \varphi_1^i(\tau)\varphi_2^k(\tau)\,\mathrm{d}\tau = (\Delta^{-1})_{ik}\,, \tag{2.12}$$

or

$$\lim_{t\to\infty}\overline{\varphi_1^i(t)\varphi_2^k(t)} = (\Delta^{-1})_{ik}\,, \tag{2.13}$$

where the bar denotes the average over the noise η. We can easily prove eq. (2.13): let us formally integrate eq. (2.11) by writing

$$\begin{aligned}\varphi_1^i(t) &= \int_0^t (\mathrm{e}^{-\Delta\tau})_{ij}\eta_j(t-\tau)\,\mathrm{d}\tau\,,\\ \varphi_2^k(t) &= \int_0^t (\mathrm{e}^{-\Delta^{\mathrm{T}}\tau})_{kl}\eta_l(t-\tau)\,\mathrm{d}\tau\\ &= \int_0^t \eta_l(t-\tau)(\mathrm{e}^{-\Delta\tau})_{lk}\,\mathrm{d}\tau\,.\end{aligned} \tag{2.14}$$

Now

$$\begin{aligned}\lim_{t\to\infty}\overline{\varphi_1^i(t)\varphi_2^k(t)} &= \lim_{t\to\infty}\int_0^t\int_0^t (\mathrm{e}^{-\Delta\tau'})_{ij}(\mathrm{e}^{-\Delta\tau''})_{lk}2\delta_{jl}\delta(\tau''-\tau')\delta\tau'\delta\tau''\\ &= \lim_{t\to\infty} 2\int_0^t (\mathrm{e}^{-2\Delta\tau})_{ik}\,\mathrm{d}\tau = (\Delta^{-1})_{ik}\,,\end{aligned} \tag{2.15}$$

and eq. (2.13) is proved.

Practically we will estimate $(\Delta^{-1})_{ik}$ from eq. (2.13) using finite time: we will integrate our equation not for an infinite time but up to $t = t_{\rm PF}$ (here $t_{\rm PF}$ plays the role of $n_{\rm PF}$ in the second-order algorithms), with a $t_{\rm PF}$ long enough for the error to be negligible.

Now we want to study numerically the Langevin system (2.11): so we will have to discretize the time. The most naive expression is

$$\varphi(n+1) = \varphi(n) + \varepsilon O\varphi(n) + \sqrt{2\varepsilon}\, r(n)\,, \tag{2.16}$$

where we omitted the euclidean space-time indices, and where O is $(-\Delta)$ for φ_1 and $(-\Delta^{\rm T})$ for φ_2, n labels the discretized Langevin time, and the $r(n)$ are random numbers with

$$\langle r(n)\rangle = 0\,, \qquad \langle r(n)^2\rangle = 1\,.$$

This naive transcription has been tested on a variety of different physical systems; it turns out that it succeeds in being a good approximation of the corresponding continuous equation only for very small integration steps ε, such that the computer time needed for the integration is prohibitively long. The way out is to consider a more accurate discrete transcription (that will ensure realistic computing time):

$$\varphi_1(n+1) = \varphi_1(n) - \varepsilon\Delta\varphi_1(n) + \tfrac{1}{2}\delta\varepsilon^2\Delta^2\varphi_1(n) + \sqrt{\varepsilon}\{(1+\tfrac{1}{2}\delta\Delta)r(n) + s(n)\}\,, \tag{2.17}$$

and the same for φ_2, with $\Delta \to \Delta^{\rm T}$. Here $r(n)$ and $s(n)$ are two independent random variables. The case in which $\delta = 1$ corresponds to a second-order Runge–Kutta approximation (for the deterministic part): this is the only case we have considered [1], although it is not clear whether a value of δ slightly larger than 1 could be better.

To end this section we note that, in the same way that we proved eq. (2.13), one can show from eq. (2.11) that, if the operator Δ is normal ($[\Delta, \Delta^*] = 0$),

$$\lim_{t\to\infty} \overline{\varphi_1^i(t)\varphi_1^k(t)^*} = 2[(\Delta + \Delta^*)^{-1}]_{ik}\,. \tag{2.18}$$

We will use this relation in sect. 3 in order to estimate the error implied from considering a finite $t_{\rm PF}$.

3. Minimizing the errors

We have seen in sect. 2 that in the method we are proposing for simulating the feedback of quark loops over the gauge field dynamics there is an intrinsic systematic error of order ρ (or order $t^{1/2}$ in the Langevin formulation, (2.4)). Assuming that ρ is small we want to estimate the error induced by the fact that $n_{\rm PF}$ (or $t_{\rm PF}$, in the Langevin pseudofermionic formalism) is finite.

Consider the complete Monte Carlo cycle for constructing $\mathrm{d}\mu_{\rm eff}[A]$ that we described in sect. 2: although not compulsory when one begins a new cycle it is convenient to use as a starting point (initial conditions for the φ-fields) the $n_{\rm PF}$th

value of the pseudofermionic variables one computed in the previous cycle. Indeed they will be off-equilibrium by a quantity proportional to ρ. For n_{PF} large enough we can write [10].

$$\frac{1}{n_{\mathrm{PF}}} \sum_{n=1}^{n_{\mathrm{PF}}} \varphi_k^{(n)*} \varphi_i^{(n)} = (\tilde{\Delta}^{-1})_{ik} + S_{ik} + R_{ik}\,, \tag{3.1}$$

where S_{ik} is a systematic effect proportional to $1/n_{\mathrm{PF}}$ and R_{ik} is a noise proportional to $(1/n_{\mathrm{PF}})^{1/2}$. The S_{ik} term would eventually be exponentially small in n_{PF} if one could approximate (Δ^{-1}) with

$$\frac{1}{n_{\mathrm{PF}}(1-x)} \sum_{n=xn_{\mathrm{PF}}}^{n_{\mathrm{PF}}} \varphi_k^{(n)*} \varphi_i^{(n)}\,, \tag{3.2}$$

where x $(0 \leqslant x < 1)$ is such that (xn_{PF}) is an integer ((xn_{PF}) is called n_{D} in sect. 2). But one should be aware that this requires very large values of n_{PF}.

In the Langevin framework (and, by using the equivalence of the small-step Monte Carlo procedure with a Langevin-like procedure, also for the Metropolis updating scheme) it is very easy to see that the global systematical error done in computing expectation values, over $\mathrm{d}\mu_{\mathrm{eff}}[A]$ will be of the form (n_{f} is the number of fermionic species)

$$\frac{\rho^2}{n_{\mathrm{PF}}} (An_{\mathrm{f}} + Bn_{\mathrm{f}}^2) + \mathrm{O}\left(\frac{1}{n_{\mathrm{PF}}^2}\right), \tag{3.3}$$

where the term proportional to n_{f}^2 comes from the noise contribution (R_{ik}) and the n_{f} part originates from the systematic effects (S_{ik}). It follows that the choice of the algorithm to be used depends on the number of fermionic species one wants to consider: if we recall that in our formulation n_{f} is not necessarily an integer number, and that the x parameter of eq. (3.2) has the role of making small the systematic error term appearing in eq. (3.1), S_{ik}, it becomes clear that x should be chosen close to one for a small n_{f} ($n_{\mathrm{f}} \to 0$), while a small x value is convenient for large n_{f}.

The last point we want to discuss here concerns the advantages presented by a heat bath (or Monte Carlo) defermionization with respect to a Langevin one, and vice versa. Let us assume we are using Kogut–Susskind fermions. We have seen that the Monte Carlo approach is based on the second-order formalism: so we expect that the time for equilibrating the pseudofermionic system, t_{eq}, will be proportional, when the bare quark mass m_{q} goes to zero, to m_{q}^{-2}. On the other hand the noise contribution to the error should not be too big. On the contrary the Langevin-like algorithm is based on a first-order formalism. In this case the diagonal term of the operator we want to equilibrate will be m_{q}, and $t_{\mathrm{eq}} \sim m_{\mathrm{q}}^{-1}$. One pays for this nice feature by the fact that

$$\overline{|\varphi_1^i|^2} = \frac{1}{m_{\mathrm{q}}}\,,$$

as can be seen from the relation (2.18), and from the fact that in the KS approach [16]

$$\Delta + \Delta^* = 2m_q\,, \tag{3.5}$$

This means that there is a noise on $\overline{\varphi_1\varphi_2}$ proportional to m_q^{-1}; it is a stronger effect than the one found in the Monte Carlo approach (numerical experiments show that the noise on the equivalent quantity stays quite small for small m_q).

We can now formulate our conclusions, by using the expression (3.3). The use of the Langevin equation is suitable for small number of flavours, while the Monte Carlo and heat bath are to be preferred for large n_f. Moreover, the value n_f^c for which it is convenient to flip from the first-order formalism to the second-order one, is a function of m_q.

As a last remark we note that in the expression (3.3) there is an overall ρ^2 factor, and that the global error is given by this expression plus the effect due to the finiteness of ρ. So it seems to us to be convenient to fix n_{PF} to a value reasonably large (for the values of the coupling constant, of the lattice size and of m_q used in ref. [1] $n_{PF} \simeq 50$ appeared to be an acceptable choice), and to extrapolate ρ to zero. This procedure is, as we noticed in subsects. 2.2, 2.3, a suitable way of avoiding an extrapolation in a two-variables space.

4. The structure of the numerical experiment

In the previous sections we have enumerated a frightening quantity of possible options, ways of extrapolating, practical differences in implementing the suggested algorithms: we have now to be clear about which are the optimal ones.

Let us start by discussing which lattice formulation we have to choose for the fermionic contribution to the effective action. In our opinion the job is best done by the KS fermions. Several advantages over Wilson fermions can be easily seen: there is manifest chiral symmetry (see the last of the references in [16] and [9]), the fermionic determinent is positive, the bare quark mass is defined on an absolute scale (due to chiral invariance the critical point of the theory has to stay at $m_q = 0$; there is not yet a value as the Wilson K_c, critical K, to be found). Moreover the corrections to the continuum limit are proportional to a^2 (where a is the lattice spacing), while on the contrary they are proportional to a in the Wilson action (in this case, due to the presence of an explicit chiral invariance breaking term, operators of dimension-5 like $\bar{\psi} D_\mu D^\mu \psi$ or $\bar{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi$ are allowed. These operators are not present in KS formulation, which preserves chiral symmetry). Last but not least in the KS formulation just one variable for the lattice site is present ("staggered fermions"), in contrast with the four spin components in the Wilson formulation; so the computer KS program turns out to be faster by a factor of order 4 than the Wilson fermion program, and occupies much less memory. On the other hand the identification of quantum numbers (spin, isospin) is straightforward for Wilson

fermions, and less simple (in particular for the baryonic sector) for KS fermions [16]. So a possibility could be to represent the *external* quark lines (Δ^{-1} in eq. (2.2)) in the Wilson picture. For the mesons, however, it costs only a slight increase of CPU time to perform the computation also using KS external lines. A separate discussion is needed for the $I=0$ part of the spectrum, and we will present it in appendix A.

Let us turn now to the practical way in which the mass spectrum computation (of a theory with $n_f=2$ or 3) should be performed. For obtaining reasonably accurate results one may have to analyze to the order of 10^2 statistically independent gauge field configurations (on a lattice with something like $10^3 \cdot 20$ sites, at squared coupling constant $g^2 \sim 1$). The number of Metropolis time steps (with optimized efficiency) needed to destroy the correlation between the estimated masses associated with two gauge field configurations is unclear. In ref. [4] masses were found to be correlated up to ~ 1000 steps; this effect is however mainly due to the influence of the boundary conditions on the fermionic Green functions in the Wilson formulation [8]. Anyhow if in a quenched computation one computes the Wilson quark correlation functions on one configuration over one hundred, the pure gauge Metropolis upgrading only takes an order of 10% of the total computer time [4, 5]; therefore if we loose a factor 10 for generating the gauge field configurations using $d\mu_{\text{eff}}[A]$, instead of the pure gauge measure $d\mu[A]$, we just need a factor 2 more of total computer time.

We can go further by using the following strategy: we upgrade the whole system (gauge fields and pseudofermions) one hundred times, using a large value of ρ, we call ρ_L (let us assume ρ_L is such that the pure gauge Metropolis procedure is optimized). This way we will produce a configuration which is slightly off-equilibrium (with respect to the measure $d\mu_{eH}[A]$): now we will equilibrate it by performing another hundred sweeps at a small ρ value, ρ_S. We will compute the Green functions only on the last configuration (of the 200 we have produced in the way we have described).

This was just a very naive sketch of a possible efficient scheme, but we can try now to improve it. Our defermionization algorithm can be thought as characterized by the three parameters ρ, $\beta = 6/g^2$ and m_q: so let us suppose our final configurations to have been obtained with the choice of the parameters $\tilde{\rho}$, $\tilde{\beta}$ and $\tilde{m}_q$ (where $\tilde{\rho}$ is small enough to make negligible the error induced by its finiteness, $\tilde{m}_q$ goes as close to zero as the size of our lattice allows it and $\tilde{\beta}$ is in the scaling region). We can think now of performing our 100 "fast" steps using the parameters ρ_F, β_F and m_q^F chosen such that

$$E(\rho_F, \beta_F, m_q^F) = E(\tilde{\rho}, \tilde{\beta}, \tilde{m}_q),$$
$$\langle\bar{\psi}\psi\rangle(\rho_F, \beta_F, m_q^F) = \langle\bar{\psi}\psi\rangle(\tilde{\rho}, \tilde{\beta}, \tilde{m}_q). \tag{4.1}$$

In this way the configuration we get at the end of our 100 fast sweeps (done with

ρ_F, β_F and m_q^F) will be as close as possible to the thermal equilibrium with $d\mu_{eff}[A]$ ($\tilde{\rho}$, $\tilde{\beta}$, $\tilde{m}_q$). We should however stress that the number $100+100$ we are quoting here is arbitrary enough; the optimal number of sweeps needed between two configurations on which the averages are done is at the moment quite unclear, and will depend on the size of the lattice.

What will be the effect of internal quark-loops on the masses? One plausible possibility is that, for the $I \neq 0$ particles and the lowest-lying baryons, it is negligible, while for the heavier states it could produce some large widths (small widths have the nice feature of simplifying the analysis of the correlation functions). Let us consider the hypothetical situation in which there already exists a very accurate computation done in the quenched approximation. This computation has been done on a large lattice, using an improved action [22] (in order to minimize the effects of the non-zero lattice spacing), and the masses have been computed with high precision (of a few percent). Now if we consider a typical mass ratio, for example

$$R = \frac{m_p}{m_\rho},$$

it is possible to expand it in powers of n_f:

$$R(n_f) = R_0 + n_f R_1 + n_f^2 R_2 + O(n_f^3).$$

Phenomenological arguments suggest that R_1 is much smaller than R_0, and that the R_2 term is negligible for $n_f = 2$; in this situation a computation of R_1 with a not-so-high accuracy (and on a not-so-large lattice) would be by fair enough. It would be very convenient to compute R_1 in a direct way by comparing the results obtained for $n_f = 0$ and $n_f = 0.1$. We should recall now what we explicitly claimed in sect. 2: our approach to the simulation of fermionic internal loops is valid also for non-integer n_f. Of course this cannot be done by comparing the results of two different Monte Carlo simulations: the statistical error would overcome the mass difference. It seems to us that what is needed is an algorithm $\mathcal{A}$ (thermalizing according to the measure $d\mu_{eff}[A]$) such that the gauge field configuration obtained by applying T times $\mathcal{A}$ to the system is a smooth function of n_f. This situation can be realized by avoiding the MC procedure, i.e. by upgrading the gauge field in the Langevin approach, and the pseudofermions by the heat bath or Langevin methods. Working at small n_f also presents the advantage that the noise contribution to the error (the R_{ik} term in eq. (3.1)), which is proportional to $\rho^2 n_f^2 n_{PF}^{-1}$ (eq. (3.3)), is in this limit negligible, and one can concentrate one's efforts in minimizing the systematic contributions to the error.

These arguments suggest that we exploit in a more systematic way the possibility of upgrading the gauge fields with a Langevin-like equation. We see two different possibilities: the first one is based on relaxing the condition that the gauge fields A are unitary, and adding to the action a term

$$\mathrm{Tr}\{(AA^* - 1)^2 + |\det(A) - 1|^2\},$$

which enforces on average the unitarity constraint. The second consists in writing a Langevin equation directly on the group manifold. In short, all we need is an upgrading algorithm producing in the phase space a trajectory that is a smooth function of the force, and satisfying the detailed balance (at least in an approximate way). We can write

$$A_\mu = \exp\{i\varepsilon^{1/2}\rho_\alpha\lambda_\alpha + \varepsilon P_A[FA_0^*]\}A_0\,, \tag{4.2}$$

with

$$F = \frac{\delta}{\delta A}(S_{\rm eff})\,.$$

where the ρ_α are gaussian random numbers, the λ_α are the SU(3) Gell–Mann matrices and P_A is the projector onto the SU(3) algebra (i.e. it picks up the traceless antihermitian part of FA_0^*). For practical purposes it is convenient to truncate the Taylor expansion of the exponential and to renormalize the new matrix to SU(3). Eq. (4.2) satisfies the detailed balance condition:

$$P(A_0, A_N) = P(A_N, A_0)\exp\{-(S_{\rm eff}[A_N] - S_{\rm eff}[A_0])\}\,, \tag{4.3}$$

(where $P(A, B)$ is the probability of transition from A to B) with an accuracy of order ε^2. Since the number of iterations grows as ε^{-1}, the effective deviations from the detailed balance turn out to be of order ε. In the limit of small ε eq. (4.2) provides an algorithm for which the trajectories are smooth functions of the parameters which appear in $S_{\rm eH}$. Multiple hitting, (updating a link more than once any time we touch it) can be used to increase the efficiency of the algorithm.

The method we are suggesting is sensible if two nearby trajectories do not separate exponentially in time. In order to see under which conditions this happens let us consider the one-variable case

$$\dot{x}(t) = -\frac{\partial U}{\partial x} + \eta(t)\,. \tag{4.4}$$

We are interested in understanding what happens to two nearby trajectories $x_1(t)$ and $x_2(t)$, which evolve under the same noise $\eta(t)$. If we set $\delta = x_2 - x_1$ we get

$$\dot{\delta} = -\left.\frac{\partial^2 U}{\partial x^2}\right|_{x=x_1(t)} \delta + O(\delta^2)\,, \tag{4.5}$$

and in the limit of small δ we see that if $\partial^2 U/\partial x^2 > 0$ the two trajectories converge, and they diverge if $\partial^2 U/\partial x^2 < 0$. It is, most of the time, in the region where $\partial^2 U/\partial x^2$ is positive (as suggested by naive arguments) the trajectories should not diverge.

The situation is completely analogous in the many-variable case:

$$\dot{x}_i(t) = -\frac{\partial S}{\partial x_i} + \eta_i(t)\,, \tag{4.6}$$

where now the crucial condition is that the average in time of the hessian matrix

$$H = \frac{\partial^2 S}{\partial x_i \partial x_j},$$

should be positive.

A serious difficulty arises if, by the symmetry of the problem, the hessian has a zero eigenvalue; in this case δ may start growing up in the direction of the correspondant eigenvector, and this could result in trajectories exponentially separating in time. Due to gauge invariance this condition is realized in gauge theories. We see three possible remedies: one is to add to the action a small term which violates gauge invariance. The second one is to fix the gauge (axial gauge) without producing ghosts. The third one consists in making after every few iterations an explicit gauge transformation over the gauge fields, in such a way as to bring them as close as possible to the identity. It seems to us that the third method should be preferred; adding a gauge breaking term to the action could badly modify the expectation value of large-distance correlation functions, and the simulation in the axial gauge converges too slowly towards thermal equilibrium. This procedure also affects the pseudofermionic sector of our cycle: we think that using the third option, also the systematic contribution in (3.1), will be diminished.

This is the computational procedure we think to be the more suitable; we obtain in this way two slightly different configurations of the gauge fields (in the sense that the trajectory in time of the values of the interesting operators stay close), respectively, let's say, with $n_f = 0$ and $n_f = 0.1$. The splitting of the masses due to the quark loops will be now free from most of the statistical errors.

We wish to thank O. Napoly for a critical reading of the manuscript and interesting discussions, and Mrs. S. Zaffanella for the very careful typing of a very tricky manuscript. The work of H.W.H. was supported by the US Department of Energy under grant no. DE-AC02-76ER02220.

Appendix A

THE $I = 0$ SECTOR

One of the goals one can try to reach by computer simulations is to obtain results about the masses of the $I = 0$ mesons; this is clearly a problem of great physical interest. It is, unluckily enough, also rather hard: one has to evaluate in this case

$$\overline{G_{ii}(A) G_{kk}(A)},$$

(where G are the fermionic Green functions) and that is very difficult. In fact to estimate the correlations one has to do an explicit average over the A field configurations, and also if i is kept fixed one has to do the computation for all k.

The simplest possibility is to use the Metropolis or Langevin to compute $G_{kk}(A)$ for all k in the quenched limit; if we set

$$M_{I=1} = m_{I=0} + \Delta m n_f + O(n_f^2) ,$$

for n_f small we get

$$\lim_{n_t = |i-k| \to \infty} \frac{G_{ii}[A] G_{kk}[A]}{G_{ik}[A] G_{ki}[A]} = \Delta m n_t . \tag{A.1}$$

This object is very difficult to evaluate for all channels except the pseudoscalar one, where the signal is rather high. A second possible way out would be to compute $G_{kk}[A]$ by means of the hopping-parameter expansion [6]. The common bottle-neck of these methods is that in practice they do not allow us to measure the signal at a distance larger than $n_t \sim 3$: this is due to the presence of a large statistical error.

Let us describe now the method we think could be applied to solve this problem*. We introduce two different pseudofermionic fields φ_1 and φ_2 (splitting the n_f fermionic species contribution to the action into two $\frac{1}{2}n_f$ equal parts), and consider the operator

$$O_\alpha(t) = \sum_{\boldsymbol{x}} \varphi_\alpha^*(\boldsymbol{x}, t) \varphi_\alpha(\boldsymbol{x}, t) , \qquad \alpha = 1, 2 , \tag{A.2}$$

where the sum over the spatial part $\boldsymbol{x}$ is done over the tth hyperplane of dimension 3. We add now to the action a term $\varepsilon O_1(t=0)$, setting ε to a small value ε_0, and measuring the quantities

$$R_\alpha(t) = \frac{1}{\varepsilon} \{ \langle O_\alpha(t) \rangle_{\varepsilon = \varepsilon_0} - \langle O_\alpha(t) \rangle_{\varepsilon = 0} \} . \tag{A.3}$$

We get in this way

$$\begin{aligned} R_1(t) &\sim e^{-m_{I=0} t_{I=0}} + e^{-M_{I=1} t_{I=1}} \\ R_2(t) &\sim e^{-m_{I=0} t_{I=0}} - e^{-M_{I=1} t_{I=1}} . \end{aligned} \tag{A.4}$$

If the mass splitting is large enough we can measure in this way $m_{I=0}$ and $M_{I=1}$. But the most important remark (and we built all this machinary just for this goal) is that if the splitting is small we get

$$\frac{R_2(t)}{R_1(t)} \sim -\Delta m t . \tag{A.5}$$

In this way it should be possible to measure also a very small splitting. The price we will have to pay is that we will have to perform a separate computation for every choice of the particle quantum numbers; but this seems to us to be the only realistic possibility.

* For the application of an analogous method to the evaluation of the glueball mass see ref. [23].

Appendix B

SCATTERING AMPLITUDES VIA MASSES FLUCTUATIONS

The way in which the particles' masses are computed in a numerical simulation is quite straightforward. For the $I \neq 0$ mesons, for example, one first computes

$$G_\Gamma(\boldsymbol{x}, t|A) \equiv \langle \psi \Gamma \psi(\boldsymbol{x}, t) \bar{\psi} \Gamma \psi(\boldsymbol{0}, 0) \rangle_A \tag{B.1}$$

and sets his operators to zero spatial momentum by defining

$$G_\Gamma(t, A) = \sum_{\boldsymbol{x}} G_\Gamma(\boldsymbol{x}, t|A) . \tag{B.2}$$

This procedure is repeated for each configuration $A^{(n)}$. Finally one computes

$$G_\Gamma(t) = \int \mathrm{d}\mu_{\mathrm{eff}}[A] G_\Gamma(t|A) , \tag{B.3}$$

and the interesting mass will be given from the large-time behavior

$$\lim_{t\to\infty} \left\{ -\frac{1}{t} \ln G_\Gamma(t) \right\} = m . \tag{B.4}$$

We can also think of defining a value of the mass for each $A^{(n)}$th configuration, by the relation

$$\lim_{t\to\infty} \left\{ -\frac{1}{t} \ln G_\Gamma(t|A^{(n)}) \right\} = m_\Gamma[A^{(n)}] . \tag{B.5}$$

Now we ask ourselves if the following relation is true:

$$\int \mathrm{d}\mu_{\mathrm{eff}}[A] m_\Gamma[A] \equiv \tilde{m}_\Gamma \overset{?}{=} m_\Gamma . \tag{B.6}$$

The answer is easily given, and it is no [25]. We will now discuss this point in some detail. Let us consider the case of a fairly large box, so that the fluctuations induced in the masses by the boundary conditions can be neglected (these fluctuations should go to zero as a high power of L), and look at the behavior of

$$G_\Gamma^{(n)}(t) = \int \mathrm{d}\mu_{\mathrm{eff}}[A] [G_\Gamma(t|A)]^n \tag{B.7}$$

in a finite large box of size L. Now we expect $G_\Gamma^{(n)}(t)$ to behave like

$$\lim_{t\to\infty} G_\Gamma^{(n)}(t) = \mathrm{e}^{-m_\Gamma^{(n)} t} , \tag{B.8}$$

where $m_\Gamma^{(n)}$ is the mass of the lightest state composed from n particles present in the box, in which each quark has different spin or flavor quantum numbers. If $m_\Gamma^{(n)}$

is an analytic function of n we have

$$\frac{\mathrm{d}}{\mathrm{d}n} m_\Gamma^{(n)}|_{n=0} = \tilde{m}_\Gamma . \tag{B.9}$$

The interaction between particles of different flavors can be expected to be attractive (van der Waals forces are generally attractive); this also follows by convexity arguments (e.g. $\overline{G^2} > \bar{G}^2$). There are two possible scenarios:

(a) particles do not form a bound state, and have an attractive scattering length L;

(b) they do form a bound state with binding energy m_B.

A simple ansatz for $m^{(n)}$ is therefore for the two cases

$$m_\Gamma^{(n)} = n m_\Gamma - \frac{n(n-1)}{2V} \frac{l}{m_\Gamma} \tag{B.10a}$$

$$m_\Gamma^{(n)} = n m_\Gamma - \tfrac{1}{2} n(n-1) m_B . \tag{B.10b}$$

These two equations follow from assuming the existence of two-body forces, and small l and Δm; the constant can be computed in the framework of non-relativistic potential models [24]. We will just use them at a very qualitative level. Using eq. (B.9) we get

$$\tilde{m}_\Gamma = m_\Gamma + \frac{1}{2V} \frac{l}{m_\Gamma} , \tag{B.11a}$$

$$\tilde{m}_\Gamma = m_\Gamma + \tfrac{1}{2} m_B . \tag{B.11b}$$

This means that there is a non-zero well-defined difference between the most probable mass (i.e. the average mass) and the true mass. In the case (a) the difference disappears when the volume of the box grows to infinity, while in case (b) there is a finite gap also for large volumes, i.e. fluctuations in the mass values do *not* go to zero when $V \to \infty$. This last one is certainly the case of the proton; moreover m_B is corresponding to the binding energy of the Ξ with a nucleon, which can be extracted from measurements on hypernuclei (hyperfragments). m_B can be estimated to be in this case less than 100 MeV, so we expect an error not greater than ~50 MeV (5 per cent) rising from computing $\tilde{m}_\mu$ instead of m_μ.

The situation can be further clarified if we write the probability distribution for the effective mass at distance t. Using the relation

$$G_\Gamma(t) = \int \mathrm{d}p_t(\mu)\, \mathrm{e}^{-\mu t} \tag{B.12}$$

and (B.10) we get

$$\mathrm{d}p_t(\mu) \propto \sqrt{\frac{t}{\Delta m \cdot \pi}} \exp\left\{ -t \frac{(\mu - \tilde{m}_\Gamma)^2}{2\Delta m} \right\} \mathrm{d}\mu , \tag{B.13}$$

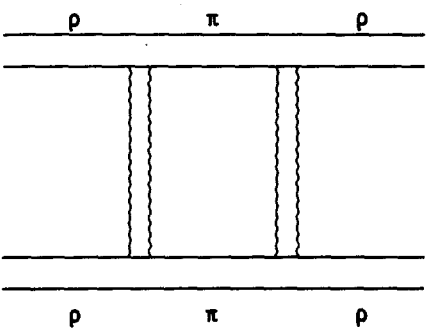

Fig. 1. The diagram dominating the two-ρ propagator large time behavior.

where for respectively the cases (a) and (b)

$$\Delta m = \frac{l}{V m_\Gamma}, \tag{B.14a}$$

$$\Delta m = m_B, \tag{B.14b}$$

It is easily seen that when $t \to \infty$ the distribution of the mass becomes very sharply peaked around the wrong value. This phenomenum is very well-known [25]. The value of m which maximizes the integral has a probability of the order $e^{-t\Delta m}$. For the protons (and likely for the other hadrons) the effect does not seem to be very important; the time t needed to resolve different resonances having the same quantum numbers is of the order of $(150\text{–}200\ \mathrm{MeV})^{-1}$, so that in the useful region $t\Delta m$ is normally a small quantity (only for unnecessarily long lattices does this effect become important). This also means that the integral (B.12) is dominated by the contributions from the center of the distribution and not from the tail, implying that it is not necessary to consider too many configurations.

Unfortunately the situation is not so nice in mesonic channels: two ρ have the same quantum numbers of two pions, so that the diagram of fig. 1 dominates the two-ρ propagator large-time behavior. This approximately means

$$G_\rho^2(t) \sim \frac{1}{V} e^{-2m_\pi t} + e^{-2m_\rho t}. \tag{B.15}$$

In other words in the ρ propagator there is a small component which behaves as $V^{-1/2} e^{-m_\pi t}$ and not as $e^{-m_\rho t}$. This effect can also be expected from naive arguments: in the presence of a background field $\bar{\psi}\gamma_\mu\psi$ excites from the vacuum a ρ and also a π with a random phase. Therefore the total probability of creating a π from the vacuum by acting with $\int_V \bar{\psi}\gamma_\mu\psi \, d_x^D$ is proportional to $V^{-1/2}$. This effect can be dangerous, but the diagrams of fig. 1 are likely to be small at the threshold.

It is clear then that a study of mass fluctuations can be seen as the analysis of the contributions of some diagrams to the scattering amplitude. Eqs. (B.11) are

particularly interesting in the case of the pion; from chiral symmetry arguments it turns out that the scattering length-squared of the pion is proportional to $m_\pi^2 f_\pi^{-4}$ so that we get

$$\tilde{m}_\pi \simeq m_\pi + \frac{1}{V f_\pi^2},$$

implying that the fluctuations of the pion mass do not increase when m_π goes to zero (on-shell pions at zero momentum are free when m_π goes to zero). This is not the case for Wilson fermions; in this formulation chiral symmetry is explicitly broken and the squared scattering length-squared is different from zero (proportional to a) for zero mass pions. Larger fluctuations are present in this case.

While the pattern of small mass fluctuations has been "experimentally" observed in the KS scheme, the opposite situation seems to hold for the Wilson formulation on small lattices (for $r = 1$, see ref. [4]). The main cause can be found in the non-zero expectation value acquired from the space loops and in the effect of the boundary conditions on the K_c [8]. Although this effect asymptotically disappears for large L, it is dominating on medium size lattices (0.5–0.8 fm*). A drastic solution in the quenched approximation would be to choose zero boundary conditions (or to sum over different Z_3 "gauge" transformations). This problem is likely to be alleviated by choosing a value of r (the Wilson chiral symmetry breaking parameter) less than one (e.g. $r = \frac{1}{2}$), and by using an improved action for the quark fields. Moreover, if the vacuum polarization quarks satisfy antiperiodic boundary conditions in space and time, the configuration in which the space and time loops are close to the identity are likely to be preferred in the $\beta \to \infty$ limit. We can conclude that it could be possible in this way to reach together the two goals of reducing the mass fluctuations to their natural size and to have interesting information about low-energy scattering amplitudes.

Appendix C

THE PSEUDOFERMIONS: COMPUTER CODES

In this appendix we want to give some details about our computer program for inserting in the Monte Carlo simulation the contribution of the fermionic determinant. We will treat here the numerical implementation of eqs. (2.9) and (2.10).

Let us remind the reader of some general features. We have defined a cycle on our system to be composed by an updating of the full lattice of link variables (gauge fields), other than by n_{PF} (number of pseudofermionic steps) sweeps on the site variables φ (pseudofermions), using as a starting point the last $\{\varphi\}$ configuration computed in the last cycle. This second part of our updating cycle has eventually

* Lattices of ~1 fm show that Z_3 effects are dramatically reduced [26].

the duty of producing the contribution to the action of the fermionic fields. When starting the next cycle (and updating the gauge fields again) we will fetch this contribution in the action we will use to update the gauge fields.

The part of the program used to update the gauge fields is different from the normal pure gauge program in one single line, in which the fermionic contribution is added to the pure gauge action: so we will describe here only the fundamental points of the computer code used to update the pseudofermions.

Let us start from a general description of our code, that is basically made up from three different phases. In the first phase, given the configuration of the gauge fields $\{A\}$ (that is the output of the first part of our cycle), and the configuration of the pseudofermions $\{\varphi\}$ (we will use as the "initial condition" the last φ-fields computed in the last cycle), we will compute the fields

$$H_i \equiv (\not{D} + m)_{ij} \varphi_j , \tag{C.1}$$

the utility of which will become clearer in the following.

The second phase has the rôle of updating the fermions, while in the third phase the contribution to the gauge action is computed (together with $\langle \bar{\varphi} \varphi \rangle$). The second phase is repeated $n_{\mathrm{PF}} \times \tilde{n}$ number of times, the third one is repeated n_{pF} times (that means that the contribution of the φ fields to the bosonic action is computed just from every $\tilde{n}$th step).

The computer memory we need is basically twice the one needed for a pure gauge simulation. If we indicate with N_c the number of colors (3), with d the number of dimensions (4), with N the number of sites per dimension (6–8), we need to store the fields

$$\begin{aligned} &A(2dN^4N_c^2), \qquad \varphi(2N^4N_c), \\ &G(2dN^4N_c^2), \qquad H(2N^4N_c). \end{aligned} \tag{C.2}$$

The value in parentheses is the amount of real numbers we need to store for every field (the 2 is just due to the fact that the fields are complex). The A's are the gauge fields, the G's are the contributions to be summed to the pure gauge action, the φ are the pseudofermions and the H's have been defined in (C.1).

The upgrading phase is very simple: one random increment $\delta\varphi^a$ is chosen, where

$$\langle \delta\varphi^a \rangle = 0, \qquad \langle \delta\varphi^{a2} \rangle = \delta , \tag{C.3}$$

and δ is turned in such a way as to optimize the convergence toward equilibrium. We note that eq. (2.8) can be read as

$$\mathrm{e}^{-\bar{\varphi}\tilde{\Delta}\varphi} = \mathrm{e}^{\bar{H}H} . \tag{C.4}$$

So

$$\Delta S = (2\,\mathrm{Re}\,H + \mathrm{Re}\,(\Delta H))\,\mathrm{Re}\,(\Delta H) + (2\,\mathrm{Im}\,H + \mathrm{Im}\,(\Delta H))\,\mathrm{Im}\,(\Delta H) . \tag{C.5}$$

A variation in the φ-field in one site will induce $(2d+1)$ variations in the H-field.

The computation of these contributions (and the knowledge of $H\forall$ the sites we have from the first phase) allows us to compute ΔS in a very straightforward way.

Now if for example we apply the Metropolis procedure, given the random number r uniformly distributed in the interval (0, 1), if $\exp\{-\Delta S\} < r$ we do not change the φ, and try again on the same site (n times) or on the next site. Otherwise we set

$$\begin{aligned} \varphi(n) &\to \varphi(n) + \delta\varphi(n) , \\ H(n) &\to H(n) + \delta H(n) , \\ H(n \pm n_\mu) &\to H(n \pm n_\mu) + \delta H(n \pm n_\mu) . \end{aligned} \tag{C.6}$$

where the fields H are changed in $2d+1$ locations.

The last duty of the code is to compute the contribution to the bosonic action (that will be averaged over n_{pF} added terms). If we write

$$S_{\mathrm{eH}} = S_{\mathrm{G}} + \tfrac{1}{4} n_{\mathrm{f}} \sum_{ij} G_{ij} U_{ij} ,$$

we will get

$$G_{ij} = \mathrm{Re}\,[\bar{H}^i(n+n_\mu)\varphi^j(n) - \bar{\varphi}^i(n+n_\mu)H^j(n)] ,$$

where μ is the direction of the link U_{ij}.

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