SCALAR DENSITIES AND BARYON MASS DIFFERENCES IN LATTICE QCDWITH WILSON FERMIONS^{*)}

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A B S T R A C T

We compute the normalization constant and the proton matrix elements of the scalar quark densities on a $10^3 \times 20$ lattice, at $\beta = 6.0$, in the quenched approximation and for three values of the Wilson parameter: $K = 0.1515, 0.1530, 0.1545$. The normalization constant is in agreement with a new Ward identity derived in this paper. In terms of the usual D and F terms of the baryon octet mass differences, we find $D/F = -0.4 \pm 0.2$, in agreement with the experimental value $(D/F)_{\text{exp}} = -0.3$. We observe that D/F decreases in absolute value for large quark mass, as suggested by the constituent quark model. Using a previous lattice determination of quark masses, we find $M_{\bar{u}} - M_u = 210 \pm 60$ MeV, to be compared with the measured value $(M_{\bar{u}} - M_u)_{\text{exp}} = 380$ MeV. We also determine the nucleon σ -term to be $\sigma = 15 \pm 4$ MeV.

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1. Introduction

Lattice QCD with Wilson fermions⁽¹⁾ provides a computational scheme to study the properties of hadronic matter in a systematic way.

Besides the hadronic spectrum, quantities related to the chiral symmetry breaking are of particular interest, since they provide a test of the field theory aspects of QCD in the fully non-perturbative regime. As shown in Ref.(2), hereafter referred to as paper I, the chiral symmetry, which is explicitly broken at the cut-off level⁽³⁾, is recovered in a very non-trivial fashion only in the continuum limit. Therefore, any test of the chiral behaviour gives an indication of how close our calculation is to the continuum limit, an information independent of and complementary to the usual tests based on the scaling behaviour of the β -function⁽⁴⁾.

A first numerical study of the chiral properties of lattice QCD has been carried out in Ref.(5), hereafter called paper II. The normalization constants of the axial and vector currents have been computed from current algebra, thereby obtaining a determination of f_π and f_ρ , and the evaluation of the bare quark masses has been given, with the pseudoscalar meson spectrum used as input [quark masses for Wilson fermions have been also determined in Ref.(6)].

In the present paper, we compute the matrix elements on the proton of the scalar quark densities, on a lattice of size $10^3 \times 20$, at $\beta = 6.0$ and in the quenched approximation. The scope

is to combine the results with the quark masses determined in II, to obtain the stable baryon mass differences and the nucleon σ -term. To this aim, a further ingredient is needed, namely the relative normalization constant of the scalar density versus the pseudoscalar one, Z_s/Z_p . As explained in I, the relative normalization can be obtained from the three-point function of the axial current with a scalar and a pseudoscalar density. In this paper, we point out that there exists a further Ward identity which says that Z_p/Z_s is equal to the derivative of the quark mass m with respect to K^{-1} (K being the Wilson hopping parameter) which was also determined in II. We have used the three-point function method to compute Z_p/Z_s . The result agrees well with $\partial m / \partial K^{-1}$, suggesting that lattice artifacts should have a small impact on our calculation.

Our results are summarized and discussed in Sect.9. We obtain the correct sign for the $\Sigma - \Lambda$ mass difference and a value for the D/F ratio quite consistent with the experimental value. On the other hand, the magnitudes of the $\Xi - P$ splitting and of the nucleon σ -term are about a factor two smaller than expected. An important source of this discrepancy may be due to the use of the quenched approximation, which implies the neglect of internal fermion loops. Finally, we see some indication that the D-coupling for the lowest-lying negative parity $1/2^-$ octet is considerably smaller than the D coupling for the stable, $1/2^+$, baryon octet.

The plan of the paper is the following. We discuss in Sect.2 the definition and the way one can compute the ratio Z_p/Z_s and

give in Sect.3 the relevant formulae relating the matrix elements we compute to the baryon mass-differences and to the nucleon σ -term. Sect.4 contains the technical details of the calculation of the correlation functions of interest and a description of the method used to extract the proton matrix elements from the correlation functions themselves.

Results are presented in Sects.5 to Sect.8. A summary and a discussion of the results are finally reported in Sect.9.

2. Scalar densities on the lattice

We discuss in this Section the relative normalization of scalar and pseudoscalar densities on the lattice.

The key result of paper I is that a non-anomalous partial conservation equation is obtained, in the continuum limit and for the non-singlet axial currents, provided we subtract properly the lattice quark mass matrix, M_0 , and rescale the naive axial current(*):

$$\langle \alpha | \nabla^\mu \hat{A}_\mu^a | \beta \rangle = \langle \alpha | \bar{q} \{ M_0 - \bar{M}, \frac{\Delta^a}{2} \gamma_5 \} q | \beta \rangle + O(a) \quad (2.1)$$

$$\hat{A}_\mu^a = Z_A A_\mu^a \quad (2.2)$$

$$A_\mu^a(x) = \frac{1}{2} \left[\bar{q}(x) \gamma_\mu \gamma_5 \frac{\Delta^a}{2} U_\mu(x) q(x+\mu) + h.c. \right] \quad (2.3)$$

$$M_0 = \frac{1}{2a} \left(\frac{1}{K} - 8 \right) \quad (2.4)$$

K is the Wilson hopping parameter and a the lattice spacing. Eq.(2.1) defines the subtracted quark mass, i.e. the analogue of the continuum quark bare mass:

$$m = M_0 - \bar{M} \quad (2.5)$$

$\bar{M}$ is itself a function of M_0 (and β). In the chiral limit,

$$\bar{M}(M_{0c}) = M_{0c}$$

(*) We denote by ∇^μ the lattice derivative $\nabla^\mu f(x) = [f(x) - f(x-\mu)] a^{-1}$

Expanding in $M_0 - M_{0c}$, we obtain:

$$m \simeq Z_m (M_0 - M_{0c}) = Z_m \frac{1}{2a} \left(\frac{1}{k} - \frac{1}{k_c} \right) \quad (2.6)$$

with:

$$Z_m = \left(1 - \frac{\partial \bar{M}}{\partial M_0} \right)_{M_0 = M_{0c}} \quad (2.7)$$

In paper II, a numerical determination of Z_A and Z_m , at $\beta = 6.0$, has been obtained:

$$Z_A = 0.85 \quad (2.8)$$

$$Z_m \simeq 0.7 \quad (2.9)$$

together with the quark mass values^(*):

$$a M_q \equiv \frac{1}{4} \left(\frac{1}{k_u} + \frac{1}{k_d} - \frac{2}{k_c} \right) = (2.5 \pm 0.3) 10^{-3} \quad (2.10)$$

$$a M_s \equiv \frac{1}{2} \left(\frac{1}{k_s} - \frac{1}{k_c} \right) = (60 \pm 7) 10^{-3} \quad (2.11)$$

$$a^{-1} = (1.84 \pm 0.23) \text{ GeV} \quad (2.12)$$

$$m = \frac{1}{2} (m_u + m_d) = Z_m M_q = (3.3 \pm 0.6) \text{ MeV} \quad (2.13)$$

$$m_s = Z_m M_s = (80 \pm 15) \text{ MeV} \quad (2.14)$$

In the present calculation we are using the same gauge configurations and quark propagators as in paper II, so that we shall use

(*) Within errors, the quark masses values in (2.10) and (2.11) agree with the results of Ref.(6).

directly the above values in what follows.

A further consequence of Eq.(2.1) is that chiral symmetry can be used to construct the lattice (composite) operators which correspond to given (composite) chiral operators in continuum QCD. In the general case⁽²⁾, this requires a mixing with operators of different naive chiral properties and equal or lower dimension. In the case of interest here, however, what is needed is simply a relative rescaling of the scalar versus pseudoscalar densities. Stated explicitly, this means that the operators^(*):

$$\hat{P}^a \equiv P^a = \bar{q} \frac{\lambda^a}{2} \gamma_5 q \quad (2.15)$$

$$\hat{S}^a \equiv \left(\frac{Z_S}{Z_P} \right) S^a = \left(\frac{Z_S}{Z_P} \right) \bar{q} \frac{\lambda^a}{2} q \quad (2.16)$$

obey, in the continuum limit, the Ward identities appropriate to the components of a (3,3) chiral multiplet with respect to the "good" axial current $\hat{A}_\mu^a$:

(*) We are assuming that flavour SU(3) is an exact symmetry at the chiral limit. Even in this case, one should introduce two different normalization constants for the octet and for the singlet scalar densities, the two constants being equal only in the quenched approximation. Since we are interested in this approximation, and in order not to complicate the notation, below we shall identify the two constants. Under the same assumptions, eq.(2.6) applies separately to each quark mass, with a unique constant Z_m , while, in general, e.g. m_{up} could also depend on the bare mass of the other quarks.

$$\begin{aligned}
 \langle \alpha | T(\nabla^\mu \hat{A}_\mu^a(x) \hat{S}^b(y)) | \beta \rangle = \\
 = \langle \alpha | T(\bar{q}(x) \{ m, \frac{\lambda^a}{2} \gamma_5 \} q(x) \hat{S}^b(y)) | \beta \rangle + \\
 - d^{abc} \delta(x-y) \langle \alpha | \hat{P}^c(y) | \beta \rangle + \dots
 \end{aligned} \tag{2.17}$$

Dots denote possible Schwinger terms, which vanish upon integration over x . To determine Z_P/Z_S in a non-perturbative way, one considers the Ward identity for the three-point functions:

$$\begin{aligned}
 \langle 0 | T(\nabla^\mu \hat{A}_\mu^a(x) S^b(y) P^c(0)) | 0 \rangle = \\
 = \langle 0 | T(\bar{q}(x) \{ m, \frac{\lambda^a}{2} \gamma_5 \} q(x) S^b(y) P^c(0)) | 0 \rangle + \\
 - d^{abd} \delta(x-y) \langle 0 | T(P^d(y) P^c(0)) | 0 \rangle \left(\frac{Z_S}{Z_P} \right)^{-1} + \\
 - d^{acd} \delta(x) \langle 0 | T(S^b(y) S^d(0)) | 0 \rangle \left(\frac{Z_S}{Z_P} \right) + \dots
 \end{aligned} \tag{2.18}$$

where dots now indicate terms which vanish upon integration over x and terms localized at $y=0$. Keeping y and z fixed and integrating upon x , eq.(2.18) gives an equation for Z_P/Z_S , which reads:

$$\begin{aligned}
 \sum_x \langle 0 | T(\bar{q}(x) \{ m, \frac{\lambda^a}{2} \gamma_5 \} q(x) S^b(y) P^c(0)) | 0 \rangle = \\
 = d^{abd} \left(\frac{Z_S}{Z_P} \right)^{-1} \langle 0 | T(P^d(y) P^c(0)) | 0 \rangle + \\
 + d^{acd} \left(\frac{Z_S}{Z_P} \right) \langle 0 | T(S^b(y) S^d(0)) | 0 \rangle
 \end{aligned} \tag{2.19}$$

We shall use eq.(2.19) to compute Z_P/Z_S , in Sect.5.

A powerful check of the whole method is given by the observation that Z_p/Z_s is equal to the constant Z_m introduced in eq.(2.6) and already computed in paper II. The reason for this shortcut is that the insertion of the unrenormalized scalar density in a Green function can be obtained by differentiating with respect to the lattice quark mass, M_0 .

Recalling that M_0 appears in the fermion action as:

$$S_F = \sum_{x,y} \bar{q}(x) K(x,y) q(y) = S_{kinetic} + \sum_x \bar{q}(x) M_0 q(x) \quad (2.20)$$

$$M_0 = M_0^a \frac{\lambda^a}{2}$$

and that the functional integration measure contains the factor $\exp(-S_F)$, we obtain the identity:

$$\sum_y \langle \alpha | T(S^a(y) \mathcal{O}_1(x) \dots) | \beta \rangle = - \frac{\partial}{\partial M_0^a} \langle \alpha | T(\mathcal{O}_1(x) \dots) | \beta \rangle \quad (2.21)$$

We apply eq.(2.21) to eq.(2.1) and obtain:

$$\begin{aligned} \sum_y \langle \alpha | T(\nabla^\mu \hat{A}_\mu^a(x) S^b(y)) | \beta \rangle = \\ = - Z_A \frac{\partial}{\partial M_0^b} \left[\frac{(M_0 - \bar{M})^c}{Z_A} \right] d^{caf} \langle \alpha | P^f(x) | \beta \rangle + \\ + \sum_y \langle \alpha | T(\bar{q}(x) \{ m, \frac{\lambda^a}{2} \gamma_5 \} q(x) S^b(y)) | \beta \rangle \end{aligned} \quad (2.22)$$

In the chiral limit,

$$Z_A \frac{\partial}{\partial M_0} \left[\frac{(M_0 - \bar{M})^c}{Z_A} \right] = Z_m \delta_{bc}$$

Comparing eq.(2.22) after integration upon x , with eq.(2.17) integrated upon x and y , we get the simple result(*):

$$Z_m = (Z_s / Z_p)^{-1} \tag{2.23}$$

(*) We thank M.Testa for this elegant proof.

3. Octet baryon mass-differences and σ -term

According to the previous discussion, the SU(3)-breaking Hamiltonian is given, on the lattice, by the scalar density^(*):

$$\begin{aligned} H_{SB} &= - \frac{(M_s - M_q)}{\sqrt{3}} \bar{q} \lambda_8 q = \\ &= - \frac{(m_s - m)}{\sqrt{3}} \left(\frac{Z_s}{Z_p} \right) \bar{q} \lambda_8 q \end{aligned} \quad (3.1)$$

The baryon matrix elements of $(\bar{q} \lambda_8 q)$, to lowest order in quark masses, are conventionally parametrized as follows:

$$\langle B' | \bar{q} \lambda_8 q | B \rangle = F \text{Tr}(B'^+ [\lambda_8, B]) + D \text{Tr}(B'^+ \{\lambda_8, B\}) \quad (3.2)$$

from which we obtain^(**):

$$M_{\Sigma} - M_p = (m_s - m) 2F = 0.379 \text{ GeV} \quad (3.3)$$

$$M_{\Sigma} + M_p - 2M_{\Sigma} = (m_s - m) 2D = -0.129 \text{ GeV} \quad (3.4)$$

(*) We recall that m is still logarithmically dependent upon the lattice spacing a . However the product $m(Z_s/Z_p) \bar{q}q$ has a well-defined, lattice-independent, limit as $a \rightarrow 0$.

(**) We use the average isospin multiplet masses (in GeV):

$$M_N = 0.939 ; M_{\Lambda} = 1.116 ; M_{\Sigma} = 1.193 ; M_{\Xi} = 1.318 ;$$

$$M_{\pi} = 0.138 ; M_K = 0.496$$

The close equality of the r.h.s. in eqs.(3.4) and (3.5) is implied by the Gell-Mann-Okubo relation.

$$-\frac{3}{2} (M_{\Sigma} - M_{\Lambda}) = (m_s - m) 2D = -0.116 \text{ GeV} \quad (3.5)$$

whence:

$$\frac{D}{F} \simeq -0.32 \quad (3.6)$$

In terms of matrix elements between proton states, we define:

$$\langle P | \bar{u}u | P \rangle = A \quad (3.7)$$

$$\langle P | \bar{d}d | P \rangle = B \quad (3.8)$$

$$\langle P | \bar{s}s | P \rangle = C \quad (3.9)$$

and a simple algebra gives:

$$A - C = 2F \quad (3.10)$$

$$A - 2B + C = 2D \quad (3.11)$$

The nucleon σ -term⁽⁷⁾ is defined as:

$$\sigma = M_q \langle P | \bar{u}u + \bar{d}d | P \rangle = m \left(\frac{Z_s}{Z_p} \right) (A + B) \quad (3.12)$$

Using the identity (2.21), one can also express the matrix element in (3.12) according to:

$$A + B = 2a \left. \frac{\partial M_p(k)}{\partial (1/k)} \right|_{k_c} \quad (3.13)$$

M_p being the proton mass. The identity (3.13) provides a useful consistency check on the values of A and B.

The determination of the σ -term, from the $I=0$ π -nucleon amplitude has been extensively discussed in the literature⁽⁷⁻¹¹⁾. We quote the value obtained in Ref.(10), which is:

$$\sigma_{exp} = 65 \pm 6 \text{ MeV} \quad (3.14)$$

The values obtained by other authors⁽⁹⁻¹¹⁾ are consistent with (3.14), although sometime errors up to a factor 3 larger are quoted.

As stated in the Introduction, we restrict ourselves to the quenched approximation, therefore ignoring internal quark loops. In this approximation (equivalent to the validity of the Zweig rule):

$$\langle P | \bar{s}s | P \rangle = C = 0$$

whence:

$$M_{\Xi} - M_p = (m_s - m) \left(\frac{Z_s}{Z_p} \right) A \quad (\text{quenched}) \quad (3.15)$$

$$\frac{D}{F} = \left(\frac{A-2B}{A} \right) \quad (\text{quenched}) \quad (3.16)$$

Within the same approximation, the nucleon σ -term is not independent of mass-differences, and it reduces to⁽¹²⁾:

$$\sigma_{\text{Zweig}} = m \left(\frac{Z_s}{Z_p} \right) (A+B) = \frac{3}{2} \frac{m}{m_s - m} \left[M_{\Xi} - M_p + \frac{1}{2} (M_{\Sigma} - M_{\Lambda}) \right] \quad (3.17)$$

$$\simeq 26 \text{ MeV}$$

where we have assumed that:

$$\frac{m}{m_s - m} \simeq \frac{M_{\pi}^2}{M_K^2 - M_{\pi}^2} \simeq 0.042$$

Suppression of strange quark loops leads to a substantial underestimate of the σ -term, as seen by comparing (3.17) with (3.14).

4. Two- and three-point correlation functions

We report in this section the technical details concerning the computation of the correlation functions and of the physical quantities, e.g. matrix elements, derived from them.

As a starting point, we have used the gauge field configurations and quark propagators of paper II, where 15 gauge configurations had been generated on a lattice of size $10^3 \times 20$, at $\beta = 6.0$, with the Metropolis algorithm (8 hits) and the Wilson action (an initial thermalization of 1500 sweeps and a separation of 120 sweeps had been allowed to suppress correlation among different configurations). Quark propagators in the quenched approximation were computed in II by solving, with the Gauss-

Seidel algorithm, the equation:

$$\sum_y K(x,y) S(y,o) = \delta_{x,o} \quad (4.1)$$

($K(x,y)$ is the kernel of the fermion action, eq.(2.20)).

Propagators have been computed for the three values of the Wilson parameter:

$$K = 0.1515, 0.1530, 0.1545 \quad (4.2)$$

We have also taken from the previous work the quark propagators with one insertion of the pseudoscalar density, needed to compute the three-point correlation function in eq.(2.19), in the calculation of Z_s/Z_p . The propagator with one γ_5 insertion is defined as:

$$S_5(x,o) = \sum_y S(x,y) \gamma_5 S(y,o) \quad (4.3)$$

and it was obtained by solving numerically an equation similar to eq.(4.1), namely:

$$\sum_y K(x,y) S_5(y,o) = \gamma_5 S(x,o) \quad (4.4)$$

using $S(x,0)$ as input.

In addition, we have computed the propagator with one scalar insertion, $S_1(x,o)$, which obeys the equation:

$$\sum_y K(x,y) S_1(y,o) = S(x,o) \quad (4.5)$$

Eq.(4.5) has been solved for the three values of K in eq.(4.2), and for all the 15 gauge configurations available. Notice that the lattice bare mass M_0 appears in the kernel in the combination [see eq.(2.20)]:

$$K(x,y) = K_{\text{kinetic}}(x,y) + M_0 \delta_{x,y}$$

By differentiating eq.(4.1) with respect to M_0 , we see that:

$$S_1(x,0) = - \frac{\partial}{\partial M_0} S(x,y) \quad (4.6)$$

The three propagators in eqs.(4.1), (4.4) and (4.5) are the basic tools to compute the correlation functions described in what follows.

i. Two- and three-point functions of quark bilinears.

We define:

$$\begin{aligned} P(t) &= \sum_{\vec{x}} \langle P_5^-(\vec{x},t) P_5^+(0) \rangle \\ P_5^+ &= \bar{u} \gamma_5 s \quad ; \quad P_5^- = \bar{s} \gamma_5 u \end{aligned} \quad (4.7)$$

$$\begin{aligned} S(t) &= \sum_{\vec{x}} \langle S^-(\vec{x},t) S^+(0) \rangle \\ S^+ &= \bar{u} d \quad ; \quad S^- = \bar{d} u \end{aligned} \quad (4.8)$$

and:

$$I_s(t) = \sum_{\vec{x}} \langle S^-(\vec{x},t) \left(\sum_{\vec{z}} \bar{s} \gamma_5 d(z) \right) P^+(0) \rangle \quad (4.9)$$

The brackets, $\langle \quad \rangle$, denote average over configurations.

The Ward identity eq.(2.19) of Sect.II reads:

$$2m I_s(t) = \left(\frac{Z_s}{Z_P} \right)^{-1} P(t) + \left(\frac{Z_s}{Z_P} \right) S(t) \quad (4.10)$$

ii. Two-point function of the proton interpolating field.

We use the non-relativistic proton field operator^(*). Defining the two component spinors^(**) χ and ξ according to:

$$q(x) = \begin{bmatrix} \chi(x) \\ \xi(x) \end{bmatrix} \quad (4.11)$$

we compute the correlation function:

$$P^{(+)}(t) = \sum_{\vec{x}, \delta} \langle P_{\delta}(\vec{x}, t) P_{\delta}^{\dagger}(0) \rangle \quad (4.12)$$

where:

$$P_{\delta}(x) = \epsilon_{\alpha\beta\gamma} \left[\chi_u^{\alpha}(x) \sigma_2 \chi_d^{\beta}(x) \right] (\chi_u^{\gamma}(x))_{\delta} \quad (4.13)$$

$P^{(+)}(t)$ is dominated by the propagation of a proton created at $t=0$, and by the propagation of the lowest negative parity state created at $t=T$, with a coupling of opposite sign⁽¹³⁾.

We have also computed the conjugated correlation function (which has a proton created at $t=T$ and the negative parity state at $t=0$):

$$P^{(-)}(t) = \sum_{\vec{x}, \delta} \langle \bar{P}_{\delta}(\vec{x}, t) \bar{P}_{\delta}^{\dagger}(0) \rangle \quad (4.14)$$

$$\bar{P}(x) = \epsilon_{\alpha\beta\gamma} \left[\xi_u^{\alpha}(x) \sigma_2 \xi_d^{\beta}(x) \right] (\xi_u^{\gamma}(x))_{\delta}$$

(*) Consistent results are obtained with the relativistic operator: $P_{rel} = \epsilon_{\alpha\beta\gamma} [u^{\alpha} C \gamma_5 d^{\beta}] u^{\gamma}$ with C the charge-conjugation matrix. As observed by previous authors^(6,13), the correlation function of P_{rel} seems to be more contaminated by higher mass states.

(**) We use Hermitian γ -matrices, with $\{\gamma_{\mu}, \gamma_{\nu}\} = 2\delta_{\mu\nu}$ and $\gamma_0 = \text{diag}(1, 1, -1, -1)$.

Using charge conjugation invariance, one sees easily that:

$$\mathcal{P}^{(-)}(t) = \mathcal{P}^{(+)}(T-t) \quad (4.15)$$

Eq.(4.15) is verified within errors in our present calculations. To improve statistics, we use the sum of the two correlation functions:

$$\mathcal{P}(t) = \mathcal{P}^{(+)}(t) + \mathcal{P}^{(-)}(T-t) \quad (4.16)$$

In the one-particle approximation, $\mathcal{P}(t)$ behaves according to:

$$\mathcal{P}(t) = Z_P e^{-M_P t} - Z_{P'} e^{-M_{P'}(T-t)} \quad (4.17)$$

iii. Three-point functions with scalar insertion.

By replacing the u or d quark propagator with S_1 , eq.(4.5), we compute the three-point functions:

$$\begin{aligned} I_u(t) = & \sum_{\vec{x}, \delta} \langle \mathcal{P}_\delta(\vec{x}, t) \left(\sum_{\vec{z}} \bar{u}u(\vec{z}) \right) \mathcal{P}_\delta^\dagger(0) \rangle + \\ & + (\mathcal{P} \rightarrow \bar{\mathcal{P}} , t \rightarrow T-t) \end{aligned} \quad (4.18)$$

$$\begin{aligned} I_d(t) = & \sum_{\vec{x}, \delta} \langle \mathcal{P}_\delta(\vec{x}, t) \left(\sum_{\vec{z}} \bar{d}d(\vec{z}) \right) \mathcal{P}_\delta^\dagger(0) \rangle + \\ & + (\mathcal{P} \rightarrow \bar{\mathcal{P}} , t \rightarrow T-t) \end{aligned} \quad (4.19)$$

and form the ratios:

$$R_u(t) = I_u(t)/\mathcal{P}(t) \quad (4.20)$$

$$R_d(t) = I_d(t)/\mathcal{P}(t) \quad (4.21)$$

Since:

$$I_u(t) = - \frac{\partial}{\partial M_{0u}} \mathcal{P}(t)$$

in the region of t where the proton state dominates we have:

$$\begin{aligned} R_u(t) &= - \frac{\partial}{\partial M_{0u}} \ln[\mathcal{P}(t)] = \\ &= \text{const} + \langle P | \bar{u}u | P \rangle t \end{aligned} \quad (4.22)$$

A linear behaviour of $R_u(t)$ indicates that we can isolate the one-particle contribution to the correlation function and determine the corresponding matrix element of $\bar{u}u$. Similarly:

$$R_d(t) = \text{const} + \langle P | \bar{d}d | P \rangle t \quad (4.23)$$

Analogous formulae hold in the region where the lowest negative parity state dominates, with $P \rightarrow P'$ and $t \rightarrow T-t$. To reduce errors, we determine the matrix elements of $\bar{u}u-2\bar{d}d$ and of $\bar{u}u+\bar{d}d$ (which give the D-coefficient for mass-differences and the σ -term, respectively) from the slope in t of the appropriate ratios:

$$R_D = \frac{I_u - 2 I_d}{\mathcal{P}(t)} \quad (4.24)$$

$$R_\sigma = \frac{I_u + I_d}{\mathcal{P}(t)} \quad (4.25)$$

Statistical errors are estimated as in the previous paper, II. Configurations are divided into three clusters, and the error for any correlation function at a given time t is estimated from the dispersion of the values of the correlation functions computed by averaging over a single cluster.

The procedure is repeated for any quantity X (mass, matrix element etc.). We fit the theoretical expression, e.g. eq.(4.17), to the correlation function of each cluster, thereby obtaining three values X_{cl} , and to the correlation function averaged over the complete set of configurations, thereby obtaining the best value $\bar{X}$. The final value for X that we quote is:

$$X = \bar{X} \pm \Delta X$$

where ΔX is computed from the dispersion of the three values X_{cl} . We will find that at $K=0.1545$ the errors are rather large, and we have various indications that single-particle saturation does not work well here for baryon states. For this reason, we will largely ignore the results at $K=0.1545$.

5. The normalization constant of scalar densities

After computing $P(t)$, $S(t)$ and $I_s(t)$, for $K=0.1515$ and $K=0.1530$, we have determined Z_p/Z_s at each given value of t by solving eq.(4.10). It is well known that $S(t)$ is much smaller than $P(t)$, due to the large mass of the scalar meson compared to the mass of the pseudoscalar one, and we have retained the root which remains finite for $S(t) \rightarrow 0$. The validity of this procedure is confirmed by the fact that the other root varies wildly with t . Fig.1 shows the values of Z_p/Z_s for $K=0.1530$ (entirely similar results are obtained for $K=0.1515$ and are not reported here for brevity). Z_p/Z_s is quite constant in t , as it should.

Taking the average value between $t=4$ and 14 , we find(*):

$$Z_p/Z_s = 0.68 \pm .01 \quad (K=0.1530) \quad (5.1)$$

$$Z_p/Z_s = 0.68 \pm .01 \quad (K=0.1515) \quad (5.2)$$

The equality of Z_p/Z_s to Z_m as determined in II, eq.(2.9), is very well supported by our results. The fact that the Ward identity eq.(2.23) is well satisfied is rather satisfactory. Note that this equation is strictly valid in the continuum limit only. The numerical agreement of (5.1) and (5.2) with (2.9) is a good indication that lattice artifacts should not affect significantly

(*) The errors given here are the dispersion of the values of Z_p/Z_s in the range $4 < t < 14$. Statistical errors at each t , computed as described in Sect.4, are much smaller.

our results. Note also that the values (5.1) and (5.2) agree with (2.9) more than they do with the perturbation theory result⁽¹⁴⁾, which is:

$$(Z_P/Z_S)_{\text{pert}} = 0.92 \qquad (5.3)$$

at $\beta = 6.0$. Detectable non-perturbative effects seem to be still present at our value of β . We do not see any appreciable mass-dependence in Z_P/Z_S , as it was found to be the case for Z_A in II, so that we can consistently take the results given above as the values at the chiral limit.

6. The proton mass

The absolute value of $\mathcal{P}(t)$, eq.(4.16), is plotted in Fig.2, for $K=0.1530$. $\mathcal{P}(t)$ changes sign from the region of small t to the region of large t , in agreement with eq.(4.17).

The figure shows clearly that the effect of negative parity states is entirely negligible for $t < 11$. There is a sensible variation of the slope for $3 < t < 5$ which indicates a sizeable contamination from positive parity higher mass states. These two features are also present at the other two values of K . If we ignore the latter problem, and fit all correlation functions in the range:

$$5 < t < 9 \quad (6.1)$$

with a single exponential, $\exp(-M_p t)$, and in the range:

$$13 < t < 16 \quad (6.2)$$

with another exponential, $\exp[-M_p'(T-t)]$, we obtain the mass values reported in Table 1 (first and third columns respectively). For comparison, we plot in Fig.3 the values of M_p thus obtained, together with the values found by Billoire et al., Ref.(13), and by Hamber [Ref.(5)] on a lattice of the same size and at the same value of β . Our mass values are somewhat higher, particularly at $K=0.1545$, but not inconsistent.

In part, the high value of M_p that we find is due to the contamination of positive parity higher mass states, which are difficult to disentangle from the proton on a small lattice such as the one we are using, particularly for small values of K^{-1} .

To substantiate the above statement, we have analyzed the same correlation functions with the following, alternative, procedure. We fit $\mathcal{P}(t)$ in the range (6.1) with the expression:

$$\mathcal{P}(t) = Z_p e^{-M_p t} + Z_{p''} e^{-M_{p''} t} \quad (6.3)$$

with $M_{p''}$ fixed to the value:

$$M_{p''} = - \ln \left[\frac{\mathcal{P}(5)}{\mathcal{P}(4)} \right] \quad (6.4)$$

We still obtain a good fit for the values of M_p listed in the third column of Table 1. The variation of M_p between the two sets, which correspond to two extreme assumptions, gives an idea of the systematic error introduced by the contamination of higher mass states.

To quote a definite value for M_p , we extrapolate linearly to the critical value K_c using only the determinations at $K=0.1515$ and 0.1530 (the value at $K=0.1545$ has a much too large systematic uncertainty). For the single particle fit, we find:

$$M_p \text{ a} = 0.80 \pm 0.12 \quad (6.5)$$

$$M_p = 1.5 \pm 0.3 \text{ GeV}$$

For the fit with eqs. (6.3) and (6.4), we find:

$$M_p \text{ a} = 0.66 \pm 0.03 \quad (6.6)$$

$$M_p = 1.2 \pm 0.2 \text{ GeV}$$

For reference, we record also the corresponding slope. For the single particle fit, we find:

$$2 \frac{\Delta M_p}{\Delta(1/k)} = 3.0 \pm 0.3 \quad (6.7)$$

while the fit with eqs.(6.3) and (6.4) gives:

$$2 \frac{\Delta M}{\Delta(1/k)} = 1.3 \pm 0.5 \quad (6.8)$$

The systematic uncertainty introduced by the higher mass, positive parity, states forbids us to reach a definite conclusion about M_p , except from the impression that M_p comes out too large in the quenched approximation. A quite smaller value of M_p is quoted in Ref.(6). However this is largely due to the assumption that M_p^2 is linear in K^{-1} . If the other assumption is made, namely that M_p behaves linearly in K^{-1} , the points of Ref.(6) would extrapolate to $M_p \simeq 0.6$ (see Fig.3), i.e. not too far from our values, eqs.(6.5) or (6.6).

The point that a $10^3 \times 20$ lattice is insufficient to separate the proton from higher mass states has been made previously by Itoh et al., Ref.(15). These authors also work with Wilson fermions, but use a renormalization-group-improved action, so that their results cannot be directly compared with ours.

7. The F and D couplings

The ratio R_u , eq.(4.20) is plotted versus t in Fig.4 (a, b and c) for the three values of K in eq. (4.2). Similarly, we give in Fig.5 (a, b and c) the ratio R_D , defined in eq.(4.24).

For $K=0.1515$ and 0.1530 , a linear behaviour in t is clearly visible, for $t \geq 4$, which allows us to determine the corresponding matrix elements. The signal is considerably worse at $K=0.1545$.

The values of the matrix elements determined from a linear fit of the form given e.g. in eq.(4.22), and in the restricted range(*):

$$4 \leq t \leq 6 \quad (7.1)$$

are reported in Table 2. To extrapolate to the chiral limit, we use only the determinations for $K=0.1515$ and $K=0.1530$, and obtain:

$$A = \langle P | \bar{u}u | P \rangle_{k_c} = 1.9 \pm 0.5 \quad (7.2)$$

$$B = \langle P | \bar{d}d | P \rangle_{k_c} = 1.4 \pm 0.2 \quad (7.3)$$

$$A - 2B = \langle P | \bar{u}u - 2\bar{d}d | P \rangle_{k_c} = -0.8 \pm 0.3 \quad (7.4)$$

(*) This restriction is unnecessary at $K=0.1515$, 0.1530 where the linear signal extends up to $t = 8$ or 9 . This makes us confident that the matrix element is not severely contaminated by higher mass states, which die around $t = 5$.

Combining with the mass values given in eqs.(2.10), (2.11), (2.12) and using the identity (2.23), we find:

$$M_{\Xi} - M_p = (M_s - M_q) A = (0.21 \pm 0.06) \text{ GeV} \quad (7.5)$$

and from the ratio of the results given in (7.4) and (7.2), we obtain:

$$\frac{D}{F} = \left. \frac{(A-2B)}{A} \right|_{k_c} = -0.4 \pm 0.2 \quad (7.6)$$

(in both cases, relative errors have been added in quadrature).

The results (7.5) and (7.6) are in qualitative agreement with the experimental values (3.3) and (3.6). In particular, the sign and magnitude of the D/F ratio are quite satisfactory. The Ξ -proton mass difference is quantitatively too small: we will come back to this point in Sect.9.

It is interesting to observe that the D/F ratio becomes smaller, in absolute value, while the quark mass increases (see Fig.6). This is in agreement with the picture derived from the constituent quark model, where the D coupling arises from gluon-mediated spin-spin forces⁽¹⁶⁾ or from SU(6) violation in the $p_z \rightarrow \infty$ frame⁽¹⁷⁾. In both cases, the D-coupling is a relativistic correction, which vanishes as the quark mass goes to infinity.

Another interesting aspect of our results concerns the negative parity states. A glance at Figs. 4 and 5 shows that the ratios have a linear behaviour also in the region $t \geq 13$. Thus one can obtain some information about the matrix elements of scalar densities also for the lowest-lying negative parity state, which should correspond to the well-established resonance⁽¹⁸⁾ N(1535). We have not tried to do this in a quantitative way. However it is

evident from the figures that while:

$$\langle P' | \bar{u}u | P' \rangle \approx \langle P | \bar{u}u | P \rangle \quad (7.7)$$

the D-coupling is much smaller, and in fact consistent with zero:

$$\langle P' | \bar{u}u - 2\bar{d}d | P' \rangle \approx 0 \quad (7.8)$$

Eq.(7.8) implies a closer Σ - Λ degeneracy for the $1/2^-$ octet, as compared to the $1/2^+$ octet. The simplest possibility for the $S=-1$ partners of the $N(1535)$ is to identify them^(16,19) with the lowest lying S-wave $\bar{K}$ -N resonances $\Lambda(1670)$ and $\Sigma(1620)$, which are indeed rather close in mass. In fact, the mass-splitting in this case could be entirely due to the mixing of the $\Lambda(1670)$ with the SU(3) singlet, $\Lambda(1405)$, which pushes up the octet, $I=0$, state. In the constituent quark model, the negative parity states are classified^(19,20) in a $(70, L=1)$ of $SU(6) \otimes O(3)$ but not much is known about their mass-differences and about the possible relations with $L=0$ baryon mass-differences. A new analysis on a larger lattice, in parallel with a study of the quark model implications for the $(70, L=1)$ states could be quite interesting.

8. The nucleon σ -term

The matrix elements of the isoscalar density for the different values of K , as determined from the ratio $R_\sigma(t)$, eq.(4.25), are reported in Table 2. Extrapolating to the chiral limit from the two determinations at $K=0.1515$, and 0.1530 , we obtain:

$$A+B = \langle P | \bar{u}u + \bar{d}d | P \rangle_{K_c} = 3.2 \pm 0.7 \quad (8.1)$$

and using the mass-value from (2.10) and (2.12) we get:

$$\sigma = M_q(A+B) = (15 \pm 4) \text{ MeV} \quad (8.2)$$

The value in (8.1) is consistent with the proton mass-slope, as given in Sect.6 and also with the slope as determined in Ref.(6). The value of σ is smaller than σ_{Zweig} , eq.(3.17), as was the case for the Ξ -P mass difference.

Note that $A+B$ is essentially constant between $K=0.1530$ and $K=0.1545$, in contrast with the apparent flattening of M_p shown in Fig.3. We interpret this as a further indication that the proton correlation function is severely contaminated by higher mass states at $K=0.1545$, which makes the single particle fit quite unreliable.

9. Summary and discussion of the results

We have presented in this paper a first, exploratory calculation of the normalization constant and of the matrix elements on the proton of the scalar quark densities in lattice QCD. Here, we summarize the results and add a short discussion of their implications, starting from the good news.

The normalization constant, Z_P/Z_S , computed from three-point functions, agrees quite well with Z_m , eq.(2.6), as required by the Ward identity eq.(2.23), in the continuum limit.

The experimental D/F ratio of the baryon octet mass differences is well reproduced: on the lattice, Σ is predicted to be heavier than Λ , which is quite a significant result. The D-coupling increases in absolute value for decreasing quark mass, as expected in the constituent quark model, where the D-coupling arises from a spin-spin interaction⁽¹⁶⁾ or from SU(6) violation in the $p_z \rightarrow \infty$ frame⁽¹⁷⁾.

We find evidence for a small D-coupling in the $1/2^-$ octet. It is intriguing to compare this with the closer degeneracy of Σ and Λ states which can be seen in the lowest-lying, $1/2^-$, states. We think that a more detailed investigation on a larger lattice could lead to definite predictions on the spectroscopy of the negative parity baryon states, about which the constituent quark model cannot say much, due to the presence of many unknown parameters.

The bad news is that the absolute size of the F coupling and of the σ -term are about a factor of two smaller than what is

needed to reproduce the Ξ -P mass-difference and the value of σ_{Zweig} , eq.(3.17) (which is what we have to compare to, working with the quenched approximation). Stated differently, if we were to use $M_{\Xi} - M_P$ and σ_{Zweig} as input to determine quark masses we would find:

$$m = \left(\frac{Z_P}{Z_S} \right) \frac{\sigma_{\text{Zweig}}}{A+B} = (5.5 \pm 0.1) \text{ MeV}$$

$$m_S = m + \left(\frac{Z_P}{Z_S} \right) \frac{M_{\Xi} - M_P}{A} = (141 \pm 4) \text{ MeV}$$

to be compared with the values given in eqs.(2.13) and (2.14), and obtained from the pseudoscalar meson spectrum.

There are a number of sources this discrepancy may come from:

- i) the presence of lattice artifacts due to a too-low value of β ;
- ii) contamination with higher-mass states;
- iii) the quenched approximation;
- iv) significant non-linear behavior in K^{-1} .

The close equality of Z_{Ξ} and Z_P/Z_S speaks against (i) and the linear behaviour of the ratios in Figs.4 and 5 suggests that perhaps (ii) should not be the dominant effect. At present, we consider (iii) and perhaps (iv) to be the most likely sources of the discrepancy. This goes well, also, with the fact that the

proton mass does come out too large and that σ_{zweig} is considerably smaller than the true σ -term. In view of these considerations, it seems crucial to repeat the calculation with dynamical fermions and for smaller values of K^{-1} .

The calculations presented in this paper have been performed with the CRAY XMP12 at CINECA, Bologna, and have required about 35 CPU hours. We acknowledge the support from the Theory Committee of INFN to obtain the necessary computing time.

Table 1.

K	$M_p(1/2^+)$		$M_p'(1/2^-)$
	(a)	(b)	
0.1515	1.10 ± 0.03	0.79 ± 0.01	1.87 ± 0.07
0.1530	1.01 ± 0.03	0.75 ± 0.01	1.78 ± 0.08
0.1545	1.00 ± 0.04	0.88 ± 0.14	1.69 ± 0.11
0.1564(K_c)	$0.80 \pm 0.12^{(i)}$ $0.92 \pm 0.04^{(ii)}$	0.66 ± 0.04	1.6 ± 0.3

Table 1. Mass of the proton and of the lowest-lying negative parity state as functions of the Wilson parameter K in units of the lattice spacing. (a): M_p obtained from a single particle fit in the region $5 \leq t \leq 9$; (b): M_p obtained with the two-particle fit, eqs.(6.3) and (6.4) of text. Last line: masses extrapolated to $K=K_c$; (i) using the values at $K=0.1515, 0.1530$; (ii) using all three values.

Table 2.

K	$A = \langle P \bar{u}u P \rangle$	$B = \langle P \bar{d}d P \rangle$	$A - 2B$	$A + B$
0.1515	1.8 ± 0.4	1.1 ± 0.3	-0.3 ± 0.1	2.9 ± 0.7
0.1530	1.8 ± 0.4	1.2 ± 0.4	-0.5 ± 0.1	3.0 ± 1.0
0.1545	1.5 ± 0.8	1.1 ± 0.4	-0.6 ± 0.1	2.6 ± 1.2
0.1564(K _c)	$1.9 \pm 0.5^{(i)}$	$1.4 \pm 0.2^{(i)}$	$-0.8 \pm 0.3^{(i)}$	$3.2 \pm 0.7^{(i)}$
	$1.5 \pm 0.5^{(ii)}$	$1.1 \pm 0.2^{(ii)}$	$-0.8 \pm 0.3^{(ii)}$	$2.6 \pm 0.6^{(ii)}$

Table 2. Matrix elements of the scalar densities as functions of K. Last line: matrix elements extrapolated to $K=K_c$; (i) using the values at $K=0.1515, 0.1530$; (ii) using all three values.

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Figure captions

- Fig.1 Z_p/Z_s versus $t+1$ at $K=.1530$.
- Fig.2 Absolute value of the proton correlation function versus $t+1$, for $K=0.1530$ (the source is located at $t=0$).
- Fig.3 Proton mass versus $1/K$ (single particle fit, see Table 1) compared to results by previous authors, Refs.(6,13).
- Fig.4 The ratio R_u , eq.(4.20) of text, versus $t+1$; (a) $K=0.1515$; (b) $K=0.1530$; (c) $K=0.1545$. The line is the best linear fit for $4 \leq t \leq 6$.
- Fig.5 The ratio R_b , eq.(4.24) of text, versus $t+1$; (a) $K=0.1515$; (b) $K=0.1530$; (c) $K=0.1545$. The line is the best linear fit for $4 \leq t \leq 6$.

- Figure 3 -

- Figure 4a -

- Figure 4b -

- Figure 4c -

- Figure 5a -

- Figure 5b -

- Figure 5c -