MONTE CARLO CALCULATION OF HADRON MASSES WITH LIGHT DYNAMICAL QUARKS

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Ground state meson and baryon masses are numerically calculated in lattice QCD with unquenched Wilson fermions on an 8^4 lattice.

The numerical calculation of the hadronic mass spectrum is one of the great challenges in lattice quantum chromodynamics. During the last years there was continuous progress in improving the calculational methods and in understanding and controlling the errors. Up to now the Monte Carlo calculations were done in the "quenched" (or "valence") approximation in which virtual quark loops are omitted (for an incomplete list of references see refs. [1–3]). The error introduced by the quenched approximation can be of the same order as the other errors investigated recently, like finite lattice size effects, effects of the lattice fermion doubling etc. Therefore it is important to study the effect of virtual loops, too.

In this letter we present the results of a calculation of the simplest hadron masses (π, ρ, p and Δ) on an 8^4 lattice, including light virtual quark loops. The Monte Carlo updating with light dynamical quarks was performed by the hopping expansion method described and tested in ref. [4]. The hadron masses were also extracted by hopping expansion using the numerical iterative procedure [2]. In order to have a direct comparison with the quenched approximation, we performed a high statistics quenched calculation on the same sized lattice at $\beta \equiv 6/g^2 = 5.70$. First we shall describe this calculation and compare it to some previous quenched calculations. Then we shall discuss some aspects of the extrapolation to zero dynamical quark mass in the unquenched case. Finally, the results with light dynamical quarks will be presented.

High statistics quenched calculation on an 8^4 lattice. For the bare coupling we have chosen the value $\beta = 5.7$, where several previous results in the quenched approximation are available. The physical size of the 8^4 lattice at this β-value is not unreasonably small, about 1.7 fm, because recent $\beta = 5.7$ string tension measurements [5,6] gave for the lattice spacing $a \cong 0.444/\sqrt{\kappa} \cong 0.21$ fm. The quark propagators were determined in 32nd order of the hopping expansion according to the "copied gauge field" method [2]. This method allows for a free (i.e. without boundary) propagation of the quarks over the periodic gauge field background and therefore eliminates a part of the finite size effects. The gauge configurations were produced by the Cabibbo–Marinari heat bath updating [7]. After 1000 equilibrating sweeps 4 initial points were chosen randomly for the determination of the quark propagators on every 50th gauge configuration. The 32nd order π- and ρ-meson propagators were built up from altogether 80 such points using the local meson operators $\bar{\psi}\gamma_5\psi$ and $\bar{\psi}\gamma_3\psi$, respectively. From 40 initial points also the proton- and Δ-propagators were constructed in the highest possible, actually 33rd,

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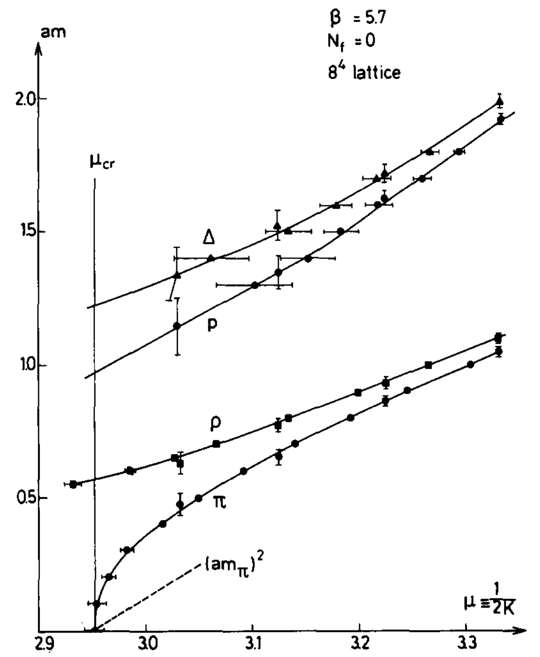

Fig. 1. The dependence of hadron masses on the quark mass parameter μ in the quenched approximation at $\beta = 5.7$ on an 8^4 lattice.

order. The local operators for the proton and Δ were $\psi(\psi^T C\gamma_5\psi)$ and $\psi(\psi^T C\gamma_3\psi)$, respectively. This quenched mass calculation took 120 CPU h on the Siemens 7.882 computer at the University of Hamburg.

The obtained dependence of the hadron masses on the bare quark mass parameter $\mu \equiv (2K)^{-1}$ is shown in fig. 1. (As usual, $K = (8 + 2am_q)^{-1} = (2\mu)^{-1}$ is the hopping parameter.) The points with horizontal error bars or, in the case of small errors, without error bars are the results of the Padé-analysis of the propagator pole position as described in ref. [2]. The points with vertical error bars give the masses obtained from the ratio of the time-slices 8/7 in the case of mesons and 6/5 in the case of baryons. The ratio of two time-slices can be determined with good accuracy from the hopping expansion, if the hopping parameter series corresponding to the two time-slices are first divided by each other and then a Padé-analysis is applied to the hopping expansion coefficients of this ratio. As can be seen, the two ways of determining the masses give consistent results. For small masses, however, the first method usually leads to smaller errors.

The results for the masses at the critical hopping parameter value

$$K_{cr} = 0.1696 \pm 0.0016\ ,$$

$$\mu_{cr} = 2.948 \pm 0.027\ , \tag{1}$$

where the pion mass vanishes, are

$$am_\rho = 0.57 \pm 0.01\ ,$$

$$am_p = 0.97 \pm 0.14 = am_\rho(1.70 \pm 0.27)\ ,$$

$$a(m_\Delta - m_p) = 0.25 \pm 0.08\ . \tag{2}$$

These numbers are, within errors, consistent with the ones obtained by the 32nd order hopping expansion on a 16^4 lattice at the same β-value [2,3]. They also agree with the findings of the Edinburgh group (Bowler et al. [1]), where the $\beta = 5.7$, 8^4 configurations were copied twice and the hadron propagators were determined by a Gauss–Seidel iteration method on the resulting $8^3 \times 16$ lattice. Our statistical errors are smaller, because these earlier calculations were based on a smaller number (between 11 and 16) of hadron propagators. The errors shown in fig. 1 have been determined from the Padé-analysis (the deviations seen in the different Padé-approximants of order 30–33). In addition, there is a relatively large configuration-to-configuration fluctuation in the horizontal position of the whole picture, which is strongly correlated to the fluctuation of the plaquette expectation value. This is expressed by the relatively large error in μ_{cr} (or K_{cr}). The shift is, however, almost entirely horizontal, i.e. the mass values at μ_{cr} are changing very little. Due to the smaller errors near μ_{cr}, the slope of the curve $(am_\pi)^2$ at μ_{cr} is now better determined than in ref. [2]. We obtained, for $(am_\pi)^2 \leqslant 0.25$,

$$(am_\pi)^2 = (44 \pm 5)(K_{cr} - K)$$

$$= (2.5 \pm 0.3)(\mu - \mu_{cr})\ . \tag{3}$$

The slope here is ~25% smaller than the one quoted in ref. [2], therefore the scale ratio between $\beta = 5.4$ and 5.7 obtained from the quark masses could be quite different from the one given in ref. [2], and therefore, might even be consistent with scaling.

The larger errors for the baryons in fig. 1 show that the Padé-table is less stable for baryons than for mesons. In fact, for the baryons there is a systematic splitting between different groups of Padé approximants: those with denominators less than, say, 12th order have a tendency of giving higher masses, whereas those with denominators higher than, say 20th order usually center around the lower end of the error bars given in fig. 1. This could be due to the effectively lower order of the hopping expansion (11th order per quark, instead of 16th order per quark for the mesons). In general, as can be seen from eq. (2), the results for the masses in the quenched approximation are unsatisfactory mainly because the proton-to-rho ratio is too large. In fact, the lattice spacing obtained from the proton mass is in agreement with the recent string tension values at $\beta = 5.7$ [5,6], but the ρ-meson mass comes out too low.

Extrapolation to zero quark mass. The hadron spectrum without heavy quark states can be described to a good approximation by massless u-, d- and s-quarks. Phenomenologically this is supported by the success of the approximate global chiral SU(3) $\times$ SU(3) symmetry. On the lattice with Wilson-fermions this implies that near the critical value of the hopping parameter $K = K_{cr}$ all hadron masses, except for the pseudo-Goldstone pseudoscalar bosons, should be slowly varying functions of the hopping parameter. This is known to be true in the quenched approximation: in fig. 1 the ρ-, p- and Δ-masses are, indeed, slowly varying near $\mu = \mu_{cr}$. Moreover, we know from previous calculations, that the physical value of the hopping parameter for the strange quarks is rather near to $K_{u,d} \cong K_{cr}$. For instance, for $\beta = 5.7$ we have [2] $K_s = 0.163^{+0.002}_{-0.006}$. Therefore, as a reasonable first approximation in a calculation with dynamical quarks one can take in the fermion determinant $N_f = 3$ massless flavours corresponding to the critical hopping parameter $K_u = K_d = K_s \equiv K_q = K_{cr}$.

The odd number of light dynamical quarks in the fermion determinant may seem dangerous for the Monte Carlo calculation, because the $N_f = 1$ fermion determinant $\det(1 - K_q M)$ could become negative for some hopping parameter values. (This danger is non-existent for an even number of degenerate flavours, because the squared $N_f = 1$ determinant is, of course, always positive.) Near $K_q = 0$ there is, however, no problem because $\det(1 - K_q M)$ is positive. Since the hopping expansion is done for the effective action $-\ln\det(1 - K_q M)$, the positivity of the fermion determinant is guaranteed as long as this expansion converges.

Compared to the quenched approximation, a complication with dynamical quarks is that the gauge configurations depend on two parameters $\beta = 6/g^2$ and $\mu_q = (2K_q)^{-1}$, instead of only on β. In the special case of massless dynamical quarks the lattice spacing is a function of one parameter, $a = a(g)$, only, since μ_q and β are related by $\mu_q = \mu_{cr}(g)$. For $\beta \to \infty$ ($g \to 0$) this dependence is given by the two-loop renormalization group formula

$$a(g)\Lambda_{latt} = (\beta_0 g^2)^{-\beta_1/(2\beta_0^2)} \exp[-1/2\beta_0 g^2] ;$$

$$\beta_0 = (4\pi)^{-2}(\tfrac{11}{3}N_c - \tfrac{2}{3}N_f) ,$$

$$\beta_1 = (4\pi)^{-4}[\tfrac{34}{3}N_c^2 - \tfrac{10}{3}N_c N_f - (N_c^2 - 1)N_f/N_c] , \quad (4)$$

here for SU(N_c) colour with N_f massless flavours. This relation holds along the curve μ_{cr} in the (β, μ_q)-plane (see fig. 2). The physically relevant curve μ_{ph}, with small but non-zero quark mass m_q is close to μ_{cr} (here we neglect, for simplicity, the mass differences of u-, d-, s-quarks). The curve μ_{ph} can be defined, for instance, by the requirement that the pion-to-proton mass ratio m_π/m_p is equal to the experimentally observed value ~ 0.148.

The other curves of constant mass ratios are parametrized by different renormalization group invariant quark mass values. In particular, for very heavy quarks ($\mu_q \gg 4$) the effect of the virtual quark loops is negligible. In this limit, for $\beta \to \infty$ the two-loop renormalization group formula (4) holds with N_f replaced by zero in β_0 and β_1. In general, the renormalization group equation in the (β, μ_q)-plane has the form (for physical quantities without wave function renormalization)

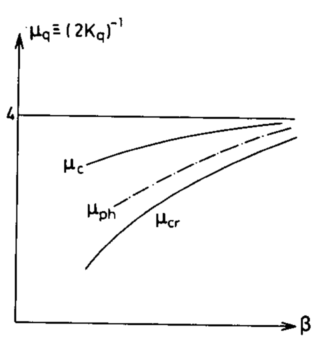

Fig. 2. The critical line with zero quark mass μ_{cr}, the physical line with small quark mass μ_{ph} and a line corresponding to some general quark mass μ_c in the (β, μ_q)-plane.

$$[-a\,\partial/\partial a + \beta_g(g,\mu_q)\,\partial/\partial g + \beta_\mu(g,\mu_q)\,\partial/\partial\mu_q]\,F = 0\,. \quad (5)$$

The differential equation for the curves $\mu_q = \mu_c(g)$ of constant physics (i.e. constant mass ratios) is

$$d\mu_c/dg = \beta_\mu(g,\mu_c(g))/\beta_g(g,\mu_c(g))\,. \quad (6)$$

Along such a curve the single variable β-function is given by $\beta_c(g) \equiv \beta_g(g,\mu_c(g))$.

The renormalization group invariant quark mass can be defined in lattice perturbation theory [8–11], but in the intermediate coupling constant range, where Monte Carlo calculations can be performed, perturbation theory is not applicable. In particular, scaling in general can be valid to a rather good accuracy in some range of coupling parameters where asymptotic scaling (corresponding to perturbation theory) is still not valid. A good example of this behaviour has recently been seen in the case of the quark–antiquark potential in SU(2) gauge theory [12]. In this intermediate range the renormalization group invariant mass $\bar{m}_q$ has, in principle, a well defined meaning, but the perturbative formulae cannot be applied to it. For practical purposes it is, however, possible to introduce $\bar{m}_q$ by, say, the lowest vector-meson mass m_{1^-} like

$$m_{1^-} = 2\bar{m}_q + E(\bar{m}_q)\,. \quad (7)$$

For heavy quarks (like c, b or t) $E(\bar{m}_q)$ can be taken, to a good approximation, from the Schrödinger equation assuming some quark–antiquark potential. For light quarks (u, d and s) we can take, as an empirical value, $E(\bar{m}_q) \cong 0.75$ GeV which agrees well with the ρ- and ϕ-meson mass. Combining this together with

$$a\bar{m}_q = \ln(1+\mu_q-\mu_{cr})$$
$$= \ln(1 + 1/2K_q - 1/2K_{cr}) \quad (8)$$

(dictated by the analogous formula for free Wilson fermions), we obtain for the lattice spacing near $\mu_q = \mu_{cr}$:

$$a \cong [am_{1^-} - 2\ln(1+\mu_q-\mu_{cr})]/0.75\ \mathrm{GeV}^{-1} \quad (9)$$

In Monte Carlo calculations we have to extrapolate from the actually measured points (β_i, μ_{qi}) $(i = 1, 2, ...)$ to the curve with zero quark mass μ_{cr}. This extrapolation is easiest if a line in the (β, μ_q)-plane is chosen, where some combination of the masses behaves linearly. Since from broken chiral symmetry we know that $(am_\pi)^2$ is linear near μ_{cr}, it is good to keep the point, where the pseudoscalar mass vanishes, fixed. According to an approximation formula [13] for the critical hopping parameter we have $K_{cr} \cong (8\sqrt{W})^{-1}$. Here $W = \frac{1}{3}\,\mathrm{Tr}\,\square$ is the one-plaquette expectation value. This suggests that a good way to choose the points (β_i, μ_{qi}) is to keep the plaquette expectation value (at least approximately) constant. One can also define in the (β, μ_q)-plane an effective β-value β_{eff} by

$$W(\beta,\mu_q) = W_0(\beta_{eff})\,, \quad (10)$$

where W_0 is the plaquette expectation value in the pure gauge theory. According to the above reasoning one should keep β_{eff} constant along the line of extrapolation.

An estimate for β_{eff} can be obtained from the approximation of the fermion determinant found in ref. [13]. With N_f flavours on an 8^4 lattice we have

$$\beta_{eff} \cong \beta + N_f(48K^4 + 2112WK^6$$
$$+ 81984\cdot 0.9937\,W^2K^8 + 3.072\cdot 10^6\cdot 0.9650W^3K^{10}$$
$$+ 1.1262\cdot 10^8\cdot 0.8784\,W^4K^{12} + ...)\,. \quad (11)$$

Here the numerical coefficients are the expansion coefficients of the free fermion effective action. The first numerical factors correspond to the infinite lattice [14] and the second factors are correcting for the 8^4 lattice.

Monte Carlo results with dynamical quarks. We determined the π-, ρ-, p- and Δ-masses in two points of the (β, μ_q)-plane. After some test runs, the points were chosen at

$$\beta = 5.4,\quad K_q = 0.163\quad (\mu_q = 3.0675\ ...):\quad \text{point A},$$
$$\beta = 5.3,\quad K_q = 0.168\quad (\mu_q = 2.9762\ ...):\quad \text{point B}. \quad (12)$$

The 8^4 lattice was first equilibrated by the pure gauge SU(3) Wilson action at $\beta = 5.6$, which roughly corresponds to the effective β-value of point A as given by eq. (11). Then the unquenched updating in the point A was started with the ratio of quark determinants calculated up to the 12th order of hopping expansion. In the first 80 sweeps the expansion coefficients were actually calculated up to 8th order and the 12th order determinants were determined by a correction factor, as described in ref. [4], using the measured correlation between the coefficients. In the last 6 sweeps genuine

Table 1
Wilson-loop expectation values $W_{ij} \equiv \frac{1}{3}$ Tr C_{ij} in the points A and B (see eq. (12) for parameters). The numbers in parentheses are the estimated errors in last numerals. In the last line the Wilson-loop expectation values on the configurations used for the quenched calculation at $\beta = 5.7$ are given.

	W_{11}	W_{12}	W_{13}	W_{22}	W_{23}	W_{33}
A	0.5298 (9)	0.2996 (12)	0.1719 (11)	0.1099 (10)	0.0428 (8)	0.0128 (7)
B	0.5428 (10)	0.3205 (12)	0.1912 (13)	0.1295 (8)	0.0546 (9)	0.0175 (9)
$N_f = 0$, $\beta = 5.7$	0.5468 (10)	0.3218 (11)	0.1922 (11)	0.1298 (8)	0.0557 (7)	0.0186 (7)

12th order determinants were taken at every link. The masses were then determined by the same method as in the quenched calculation, choosing 10 random initial points for the 32nd order quark propagators on each of the last 5 configurations. Besides, a large number of planar and non-planar Wilson loops were measured on the same configurations, in order to obtain information on the static energy of an external quark–antiquark pair. The expectation values of the simplest Wilson-loops are given in table 1. We checked in both points that the off-axis Wilson loops are, to a good approximation, consistent with the rotation invariance of the static energy, suggesting that points A and B are in the scaling region. More results on the static q$\bar{\text{q}}$-energy will be given in a later publication [15].

The obtained hadron masses, as a function of the quark mass parameter $\mu = (2K)^{-1}$ in the quark propagators, are shown in fig. 3. In the point, where the quark mass in the determinant and in the propagators coincide: $\mu_q = \mu = (0.326)^{-1}$ (i.e. in point A of the (β, μ_q)-plane) we have

$$am_\pi = 0.69 \pm 0.01\,, \quad am_\rho = 0.95 \pm 0.01\,,$$

$$am_p = 1.62 \pm 0.02\,, \quad am_\Delta = 1.74 \pm 0.02\,. \qquad (13)$$

These numbers correspond to some non-zero quark-mass (about $\bar{m}_q \cong 70$ MeV, as we shall see later), therefore they cannot immediately be compared to the quenched results eq. (2). At a qualitative level one can, however, see that the ρ-curve lies relatively higher in fig. 3 than in fig. 1. Comparing eq. (13) e.g. to the point $\mu = 3.126$ in fig. 1, which has the same distance to the critical point with $m_\pi = 0$, the value of $(m_\rho - m_\pi)/m_\pi$ is there 0.164, whereas in eq. (13) it is 0.377. The p/ρ mass ratio is also somewhat smaller (about 5%) in eq. (13) than at $\mu = 3.126$ in fig. 1.

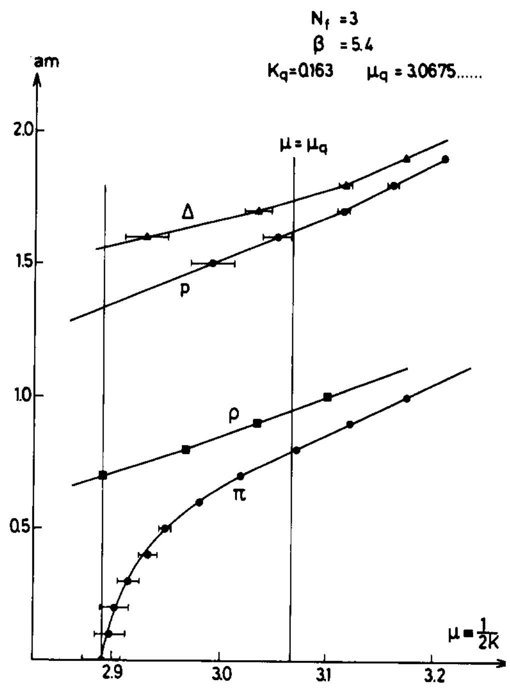

Fig. 3. The hadron masses as a function of the quark mass μ in the propagators at $\beta = 5.4$ and $\mu_q = (0.326)^{-1}$.

Therefore, the effect of virtual quark loops corrects the quenched approximation in the right direction. A more quantitative statement can, however, be made only if more information in the (β, μ_q)-plane is available (for instance, for the lattice spacing, quark mass etc.).

For the updating in our second point (point B in eq. (12)), we started with the last configuration in point A repeating the same procedure as before, with 80 + 6 sweeps and measuring the masses. The obtained Wilson-loop expectation values are given in table 1, and the masses for $\mu = \mu_q = (0.336)^{-1}$ are:

$$am_\pi = 0.3^{+0.1}_{-0.2}\,, \quad am_\rho = 0.65 \pm 0.05\,,$$

$$am_\mathrm{p} = 0.85 \pm 0.15\,, \quad a(m_\Delta - m_\mathrm{p}) = 0.24 \pm 0.09\,. \tag{14}$$

The larger errors here are due to the fact that μ_q is almost equal to the critical value μ_cr, where the pion mass vanishes. In addition to the larger errors of the masses near μ_cr, our approximation to the quark determinant is also deteriorated somewhat, in comparison to point A. There the estimated average error of the determinant ratios is less than 10% in the first 80 sweeps, and less than 6% in the last 6 sweeps. In point B the corresponding error estimates are, respectively, about 15% and 10%. Therefore, point B lies, within our errors, on the critical line μ_cr with zero quark mass. Using this information, the non-perturbative quark mass and the lattice spacing can be obtained in both points from eqs. (8), (9):

$$\bar{m}_\mathrm{q}(\text{point A}) \cong 70 \text{ MeV}\,,$$

$$a(\mathrm{A}) = (1.08 \pm 0.06)\ \mathrm{GeV}^{-1}\,,$$

$$\bar{m}_\mathrm{q}(\text{point B}) \cong 10 \text{ MeV}\,,$$

$$a(\mathrm{B}) = (0.87 \pm 0.09)\ \mathrm{GeV}^{-1}\,. \tag{15}$$

Assuming the validity of eq. (4) in point B would mean $\Lambda_\mathrm{latt}(N_\mathrm{f} = 3) = (1.5 \pm 0.3)$ MeV or [16,17] $\Lambda^\mathrm{mom}_{\alpha=1} = (160 \pm 30)$ MeV.

In conclusion, first of all we would like to stress that the present calculation demonstrates the possibility of the numerical determination of hadron masses with light dynamical quarks. The required amount of computer time is large but not prohibitive: the updating for the two points (A and B) took about 190 CPU h on the CYBER 205 at the University of Karlsruhe, and the mass determination on the configurations required, in addition, about 150 CPU h on the Siemens 7.882 at the University of Hamburg. The results in point A with quark mass $\bar{m}_\mathrm{q} \cong 70$ MeV show, that the effect of light dynamical quarks decreases the p/ρ mass ratio and increases the spin splitting. The mass values in point B, corresponding to $\bar{m}_\mathrm{q} \cong 10$ MeV, are in agreement with the experimental numbers, although the errors are still somewhat large to draw a definite conclusion. A striking consequence of eq. (15) is the relatively fast change of the lattice spacing within a rather small range of hopping parameter values: for instance, for fixed $\beta = 5.4$ this could mean more than a factor 1.5 change between $K = 0.163$ ($\bar{m}_\mathrm{q} \cong 70$ MeV) and $K = 0.167$ ($\bar{m}_\mathrm{q} \cong 0$ MeV).

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