ESTIMATE OF THE EFFECT OF VIRTUAL QUARK LOOPS ON MESON MASSES IN LATTICE QCD

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Received 11 August 1983

The 0^- and 1^- meson masses are calculated in SU(2) lattice gauge theory at $\beta = 2.3$ with Wilson fermions on a 10^4 lattice. The calculation is based on a 32nd order hopping parameter expansion. The fermion determinant can be taken into account for quark masses heavier than ~600 MeV. For lighter quarks only an estimate is given due to the limitations of statistics.

An important step in the numerical evaluation of lattice QCD [1] is the calculation of hadron masses. In the first attempts of hadron spectrum calculation [2–4] the effect of dynamical (virtual) quark loops was neglected ("quenched- or "valence"-approximation). From the point of view of numerical computation this is an important simplification, because the virtual quark loops are contained in the "fermion determinant" which is very hard to take into account in the Monte Carlo updating procedure. It turned out that the results in the quenched approximation are quite reasonable, especially in the recent calculations done on larger lattices [5,6]. This implies that the effect of dynamical quarks on the hadron masses cannot be very large. Nevertheless, it is obviously important to check this point in a calculation taking into account the fermion determinant. A first step in this direction was a recent calculation at negative flavour numbers (that is, replacing fermionic quarks by bosonic quarks in the determinant) [7], which showed only small changes in the hadron mass ratios, indeed. The extrapolation to the physical flavour number is, however, non-trivial and was, up to now, not attempted.

The quark determinant can be taken into account by several methods like the pseudo-fermion method [8], stochastic method [9] or the method of hopping parameter expansion [10,11]. In fact, in the 10th order hopping parameter expansion of ref. [11] the quark determinant was included. Its effect on the hadron masses was shown to be small, but a 10th order expansion is obviously too low for drawing a firm conclusion. By the use of the iterative method [12,6] the hopping parameter expansion can, however, be extended to much higher orders.

In the present letter a first calculation of meson masses is reported including the effect of virtual quark loops in a high (32nd) order hopping parameter expansion. For dealing with the fermion determinant the experience gained in a recent calculation of the screened quark–antiquark potential [13] was important. In fact, the 20 SU(2) gauge configurations on 10^4 lattices are identical to those used in ref. [13] for the measurement of Wilson loops.

The hopping parameter expansion coefficients of the meson propagators were determined in the "periodic box" as described in ref. [12], that is, imposing periodic boundary conditions on both the gauge- and quark fields. This does not allow to search directly for particle poles at real energy values as in the "copied gauge field method" [11,12], because the periodicity of the quark fields is strongly reflected in the expansion coefficients and this restricts the momentum values to discrete euclidean points. Therefore, I first calculated the values of meson propagators for euclidean momenta $ap_{1,2,3} = 0, ap_4 = \pi l/5$ $(l = 0, \pm 1, \ldots, \pm 5)$

[1] Supported by Bundesministerium für Forschung und Technologie, Bonn, Fed. Rep. Germany.

corresponding to periodicity. At a given hopping parameter (K) the Padé table obtained from the expansion coefficients was used to calculate the amplitude and the resulting values were Fourier transformed to configuration space in order to determine the time slices of meson propagators. The masses were then extracted, as usual, from the exponential fall-off at the largest distances. Because of the statistical errors on time slices, it turned out necessary to average first order the 24th to 32nd order Padé approximants and determine the masses from the averages. (A similar method was used also in ref. [14].) The hopping parameter expansion coefficients of meson propagators were calculated upon 32nd order from 5 initial points on each of the 20 configurations and, in order to increase the lower statistical accuracy of the low order coefficients, up to 24th order from another 20 initial points. These 25 initial points per configuration were selected randomly from the points of the 10^4 lattice. The SU(2) gauge configurations themselves were created by the Metropolis updating method. In 5 independent streams of configurations the consecutive ones were separated by 50 sweeps with 3 hits per link.

The calculation of the quark determinant in the 32nd order hopping parameter expansion was done in the same way as in ref. [13]. Let us recall that the quark part of the Wilson action is

$$S_{\mathrm{f}} = \sum_x \Big(\tilde{\psi}_x \psi_x - K \sum_\mu \tilde{\psi}_{x+\hat{\mu}} U[x,\mu](1+\gamma_\mu)\psi_x \Big)$$

$$\equiv \sum_{x,y} \tilde{\psi}_x Q_{xy} \psi_y \,. \tag{1}$$

Here ψ_x, $\tilde{\psi}_x$ denote the anticommuting quark fields on the lattice point x, $U[x, \mu]$ is the gauge field variable sitting on the link $x \to x + \hat{\mu}$ ($\mu = \pm 1, \pm 2, ..., \pm 4$) and $\gamma_\mu = -\gamma_{-\mu}$ are hermitian Dirac-matrices. Writing the "quark matrix" as $Q \equiv 1 - KM$, the hopping parameter expansion of the quark determinant can be written (for one quark flavour) as

$$\det Q = \det(1 - KM)$$

$$= \exp\Big(-\sum_{j=4}^{\infty} \frac{K^j}{j} \sum_x \mathrm{Tr}(M^j_{xx}) \Big) \,. \tag{2}$$

Here the trace-sum over lattice points is explicitly written out, therefore Tr(...) means only colour-and Dirac-traces. The hopping matrix $M_{x_1 x_2}$ is according to eq. (1)

$$M_{x_1 x_2} = \sum_{x,\mu} (1+\gamma_\mu) U[x,\mu]\, \delta_{x_1, x+\hat{\mu}}\, \delta_{x, x_2} \,. \tag{3}$$

The first non-vanishing term ($j = 4$) in the hopping parameter expansion of the effective action $S_{\mathrm{q}}^{\mathrm{eff}} \equiv -\ln \det Q$ has the same form as the pure gauge Wilson action. After performing the Dirac-trace calculation this term looks like

$$S_{\mathrm{q}}^{\mathrm{eff}}(j=4) = -16 K^4 \sum_{\Box} \mathrm{Tr}\, U_{\Box} \,. \tag{4}$$

Here $\Sigma_{\Box}$ denotes a sum over plaquettes. $S_{\mathrm{q}}^{\mathrm{eff}}(j = 4)$ can be included in the pure gauge action by a shift $\Delta\beta = 32 K^4$ ($\beta = 4/g^2$). The Monte Carlo updating of the gauge configurations was done in our case at a fixed value $\beta = 2.3$, therefore the omission of the $j = 4$ term in $S_{\mathrm{q}}^{\mathrm{eff}}$ means, that the calculation is performed at a K-dependent value of the gauge coupling constant

$$\beta_K = 2.3 - 32 K^4 \,. \tag{5}$$

At $\beta = 2.3$, $S_{\mathrm{q}}^{\mathrm{eff}}(j = 4)$ takes into account a substantial part of the quark effective action $S_{\mathrm{q}}^{\mathrm{eff}}$. (A further improvement in this direction would be to include also the $j = 6$ term in eq. (2) in the updating.)

The sum Σ_x over the lattice points for the rest

$$S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6) \equiv S_{\mathrm{q}}^{\mathrm{eff}} - S_{\mathrm{q}}^{\mathrm{eff}}(j=4) \tag{6}$$

of the effective action is evaluated only approximately by choosing a random sample of 300 points (out of the 10 000) on every configuration. As noted in ref. [13], in the expectation values only the deviation of $S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6)$ from its average $[\bar{S}_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6)]$ appears, therefore one has to determine the expansion coefficients of

$$\Delta S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6) = S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6) - \bar{S}_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6) \,. \tag{7}$$

On a given configuration these are then used to calculate, for different hopping parameters, the value of

$$\det{}_6(\Delta Q) \equiv \exp[-\Delta S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6)] \,. \tag{8}$$

In the interesting range $K \leq 0.15$ usually a good value is obtained for $\Delta S_{\mathrm{q}}^{\mathrm{eff}}(j \geq 6)$ already from the 32nd order series. This can, however, be further improved by taking, instead of the series, some of the highest order central Padé-approximants. The expectation value of some quantity F is then given as a weighted average over the configurations:

$$\langle F \rangle = \frac{\Sigma_U F[U] \det_6 (\Delta Q[U])}{\Sigma_U \det_6 (\Delta Q[U])} . \tag{9}$$

The main limitation of the present method comes from the fact that the range of values of $\det_6(\Delta Q)$ becomes larger for increasing hopping parameters (and hence for lighter quarks). Therefore, in eq. (8) at large K only very few configurations give a substantial contribution. As a consequence, the statistics become very poor. In the present case this limits the hopping parameter values to $K \lesssim 0.145$, where the pion mass is greater than ~1 (in lattice units).

Before discussing the effects of virtual quark loops, let us consider the 0^- and 1^- meson masses for $\beta = 2.3$ in the quenched approximation (that is, replacing $\det Q$ by 1). The $20 \cdot 5 = 100$ 32nd order initial points plus the $20 \cdot 20 = 400$ 24th order initial points represent, in this case, a very good statistics. The obtained masses are shown in fig. 1. For the critical value of the hopping parameter (K_{cr}), where the pion mass vanishes, a linear extrapolation of $(am_\pi)^2$ to zero gives

$$K_{cr} = 0.156 \pm 0.002 . \tag{10}$$

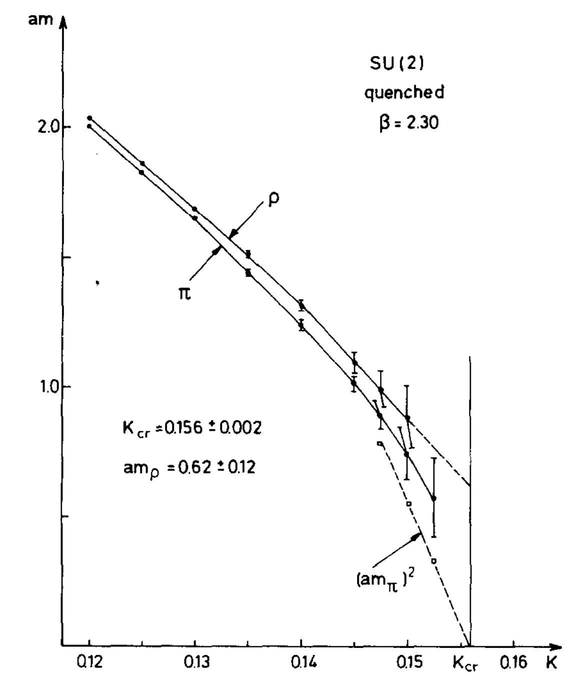

Fig. 1. The π- and ρ-meson masses as a function of the hopping parameter K in the quenched approximation at $\beta = 2.3$. The dashed line with open squares is the linear extrapolation of $(am_\pi)^2$ to zero. The ρ-meson mass is extrapolated linearly from the last measurable points to $K = K_{cr}$.

At this K-value the ρ-meson mass is

$$am_\rho = 0.62 \pm 0.12 . \tag{11}$$

From the physical ρ-meson mass it follows

$$a(N_f = 0, \beta = 2.3) = (0.80 \pm 0.16)\,\mathrm{GeV}^{-1} \simeq 0.16\,\mathrm{fm} .$$

This value has to be compared to the one obtained from the string tension: $a \simeq 1.1\ \mathrm{GeV}^{-1}$ [15,16]. Therefore, the meson masses give a smaller physical lattice spacing than the string tension, similarly to the recent calculations in SU(3) on large lattices [5,6]. {Note that the correlation length at $\beta = 2.3$ is roughly equal to 1a, similarly to $\beta = 5.7$ in SU(3) considered in ref. [6]. An earlier SU(2) calculation on a smaller ($5^3 \times 10$) lattice [17] gave at $\beta = 2.3$ $K_{cr} = 0.162^{+0.002}_{-0.001}$ and $am_\rho = 0.80 \pm 0.08$.}

The result for the π- and ρ-meson masses, which is obtained by applying eq. (9) to the hopping parameter expansion coefficients, is shown in fig. 2. As discussed

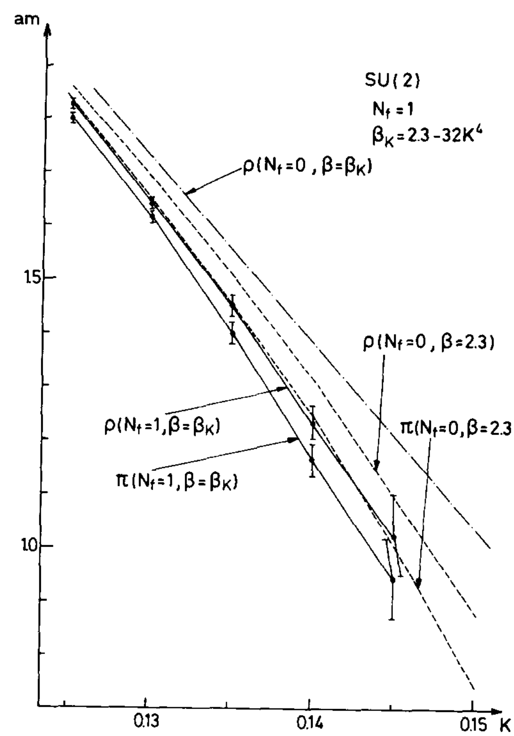

Fig. 2. The π- and ρ-meson masses for one flavour ($N_f = 1$) in the quark determinant at a K-dependent β-value $\beta = \beta_K \equiv 2.3 - 32\,K^4$ (full lines). For comparison, the curves in fig. 1 are shown by dashed lines ($N_f = 0$ and $\beta = 2.3$). The dashed–dotted line is an estimate of the ρ-meson mass at $\beta = \beta_K$. (The shift from $\beta = 2.3$ is estimated by using the β-dependence measured in ref. [17].)

before, the gauge coupling constant depends on the hopping parameter according to eq. (5). In order to see the net effect of the quark determinant one should compare the results to the masses in the quenched approximation at the same coupling constant value, that is at $\beta = 2.3 - 32\, K^4$. This can be done by shifting the $\beta = 2.3$ curves in fig. 1 by an amount corresponding to the small shift in β. A possibility is to use the results at $\beta = 2.2, 2.3, 2.4$ obtained by Fukuta et al. [17]. (See fig. 2.)

The present method does not allow to go with the quark determinant calculation to K-values above $K \simeq 0.145$. This roughly corresponds to a bare quark mass $m_q \simeq 0.6$ GeV. The only possibility is to try some extrapolation. An (ad hoc) linear extrapolation of the deviation from the $N_f = 0, \beta = 2.3$ curve gives for the critical K-value

$$K_{cr}(N_f = 1, \beta = \beta_K) \simeq 0.154 \,. \qquad (13)$$

The $\rho - \pi$ mass splitting (in lattice units) is in the measured points almost equal to the quenched $\rho - \pi$ mass splitting at $\beta = 2.3$ (see fig. 2). This gives for the ratios of lattice spacings (extrapolated to zero quark mass):

$$a(N_f = 1, \beta = \beta_K)/a(N_f = 0, \beta = 2.3) = 0.9 \pm 0.4 \,. \quad (14)$$

Using the perturbative ratios of SU(2) Λ-parameters [18,19]:

$$\Lambda_{mom}^{(N_f=0)}/\Lambda_{latt}^{(N_f=0)} = 57.4 \,, \quad \Lambda_{mom}^{(N_f=1)}/\Lambda_{latt}^{(N_f=1)} = 61.4 \,. \qquad (15)$$

Eq. (14) implies, with large errors

$$\Lambda_{mom}^{(N_f=1)}/\Lambda_{mom}^{(N_f=0)} \simeq 0.7 \,. \qquad (16)$$

The direction of shift of the critical K-value given by eqs. (10), (13) is opposite to the one observed by Daffy et al. [7] at $N_f = -2$ [in SU(3)]. This is, therefore, consistent with the simplest flavour extrapolation, although a linear extrapolation in N_f seems generally not allowed [13]. The other observation in ref. [7] is the antiscreening of the wave functions at the origin for negative flavour numbers. The expected screening for positive N_f would mean that, for instance, the vector meson coupling constant f_v^{-1}, defined by

$$\langle 0 | \widetilde{\psi}(0) \gamma_\mu \psi(0) | v(p, \sigma) \rangle = (m_v^2/f_v) \epsilon_\mu(p, \sigma) \,, \qquad (17)$$

should become smaller. This tendency is confirmed by the present calculation, although the measured effect (for $K \leqslant 0.145$) is not large. For instance, at $N_f = 0, \beta = 2.3$ and $K = 0.145$ we have $f^{-1} \simeq 0.19$, whereas for $N_f = 1, \beta = \beta_K$ and $K = 0.145$ the result is $f_\rho^{-1} \simeq 0.16$. Due to the increase of f_v^{-1} as a function of K, if extrapolated to $K = K_{cr}$, this value is still somewhat (about a factor 1.3) larger than the measured one: f_ρ^{-1} (experimental) = 0.19.

All the above estimates apply, of course, to the theoretical world with SU(2) colour and $N_f = 1$ light flavour. Using the experience gained during these calculations, the physical case with SU(3) colour and $N_f = 2$ or 3 seems, however, entirely within reach. I hope to complete this calculation in the near future.

It is a pleasure to thank P. Hasenfratz and H. Joos for discussions. I am grateful to the DESY computer division for kindly supporting this calculation, which took about 150 hours CPU time on the IBM 3081.

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