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Electromagnetic Splittings and Light Quark Masses in Lattice QCD

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Abstract

A method for computing electromagnetic properties of hadrons in lattice QCD is described and preliminary numerical results are presented. The electromagnetic field is introduced dynamically, using a noncompact formulation. Employing enhanced electric charges, the dependence of the pseudoscalar meson mass on the (anti)quark charges and masses can be accurately calculated. At $\beta = 5.7$ with Wilson action, the $\pi^+ - \pi^0$ splitting is found to be 4.9(3) MeV. Using the measured $K^0 - K^+$ splitting, we also find $m_u/m_d = .512(6)$. Systematic errors are discussed.

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If a fundamental theory of quark masses ever emerges, it may be as important to resolve the theoretical uncertainty in the light quark masses as it is to accurately measure the top quark mass. Moreover, an accurate determination of the up quark mass might finally resolve the question of whether nature avoids the strong CP problem via a massless up quark. The particle data tables [1] give wide ranges for the up ($2 < m_u < 8$ MeV) and down ($5 < m_d < 15$ MeV) quarks, while lowest order chiral perturbation theory [2, 3, 4] gives $m_u/m_d = 0.57 \pm 0.04$. Numerical lattice calculations provide, in principle, a very precise way of studying the dependence of hadron masses on the lagrangian quark mass parameters[5]. However, the contribution to hadronic mass splittings within isomultiplets from electromagnetic (virtual photon) effects is comparable to the size of the up-down quark mass difference. Thus an accurate determination of the light quark masses requires the calculation of electromagnetic effects in the context of nonperturbative QCD dynamics. In this letter, we discuss a method for studying electromagnetic effects in the hadron spectrum. In addition to the SU(3) color gauge field, we introduce a U(1) electromagnetic field on the lattice which is also treated by Monte Carlo methods. The resulting SU(3)×U(1) gauge configurations are then analyzed by standard hadron propagator techniques.

The small size of electromagnetic mass splittings makes their accurate determination by conventional lattice techniques difficult if the electromagnetic coupling is taken at its physical value. One of the main results of this paper is to demonstrate that calculations done at larger values of the quark electric charges (roughly 2 to 6 times physical values) lead to accurately measurable electromagnetic splittings in the light pseudoscalar meson spectrum, while still allowing perturbative extrapolation to physical values.

The strategy of the calculation is as follows. Quark propagators are generated in the presence of background SU(3)×U(1) fields where the SU(3) component represents the usual gluonic gauge degrees of freedom, while the U(1) component incorporates an abelian photon field (with a noncompact gauge action) which interacts with quarks of specified electric charge. All calculations are performed in the quenched approximation and Coulomb gauge is used throughout for both components. Quark propagators are calculated for a variety of electric charges and light quark mass values. The gauge configurations were generated at $\beta = 5.7$ on a $12^3 \times 24$ lattice. 200 configurations each separated by 1000 Monte Carlo sweeps were used. In the results reported here, we have used four different values of charge given by e_q =0, -0.4, +0.8, and -1.2 in units in which the electron charge is $e = \sqrt{4\pi/137} = .3028\ldots$.

For each quark charge we calculate propagators for three light quark mass values in order to allow a chiral extrapolation. From the resulting 12 quark propagators, 144 quark-antiquark combinations can be formed. The meson propagators are then computed and masses for the 78 independent states extracted.

Once the full set of meson masses is computed, the analysis proceeds by a combination of chiral and QED perturbation theory. In pure QCD it is known that, in the range of masses considered here, the square of the pseudoscalar meson mass is quite accurately fit by a linear function of the bare quark masses[6]. We have found that this linearity in the bare quark mass persists even in the presence of electromagnetism. For each of the charge combinations studied, the dependence of the squared meson mass on the bare quark mass is well described by lowest order chiral perturbation theory. Thus we write the pseudoscalar mass squared as

$$m_P^2 = A(e_q, e_{\bar{q}}) + m_q B(e_q, e_{\bar{q}}) + m_{\bar{q}} B(e_{\bar{q}}, e_q) \tag{1}$$

where $e_q, e_{\bar{q}}$ are the quark and antiquark charges, and $m_q, m_{\bar{q}}$ are the bare quark masses, defined in terms of the Wilson hopping parameter by $(\kappa^{-1} - \kappa_c^{-1})/2a$. (Here a is the lattice spacing.) Because of the electromagnetic self-energy shift, the value of the critical hopping parameter must be determined independently for each quark charge. This is done by requiring that the mass of the neutral pseudoscalar meson vanish at $\kappa = \kappa_c$, as discussed below. The results for the neutral pseudoscalars are shown in Figure 1. For the physical values of the quark charges, we expect that an expansion of the coefficients A and B in (1) to first order in e^2 should be quite accurate. For the larger values of QED coupling that we use in our numerical investigation, the accuracy of first order perturbation theory is less clear: in fact, a good fit to all our data requires small but nonzero terms of order e^4, corresponding to two-photon diagrams. Comparison of the order e^4 terms with those of order e^2 provides a quantitative check on the accuracy of QED perturbation theory. We have tried including all possible e^4 terms in the fit, but only retained those which significantly reduce the χ^2 per degree of freedom.

According to a theorem of Dashen [7], in the limit of vanishing quark mass, the value of m_P^2 is proportional to the square of the total charge. Thus, we have also allowed the values of the critical hopping parameters for each of the quark charges to be fit parameters, requiring that the mass of the neutral mesons vanish in the chiral limit. Thus A takes the form $A^{(1)}(e_q + e_{\bar{q}})^2$ to order e^2. (Order e^4 terms were not found unnecessary to fit the

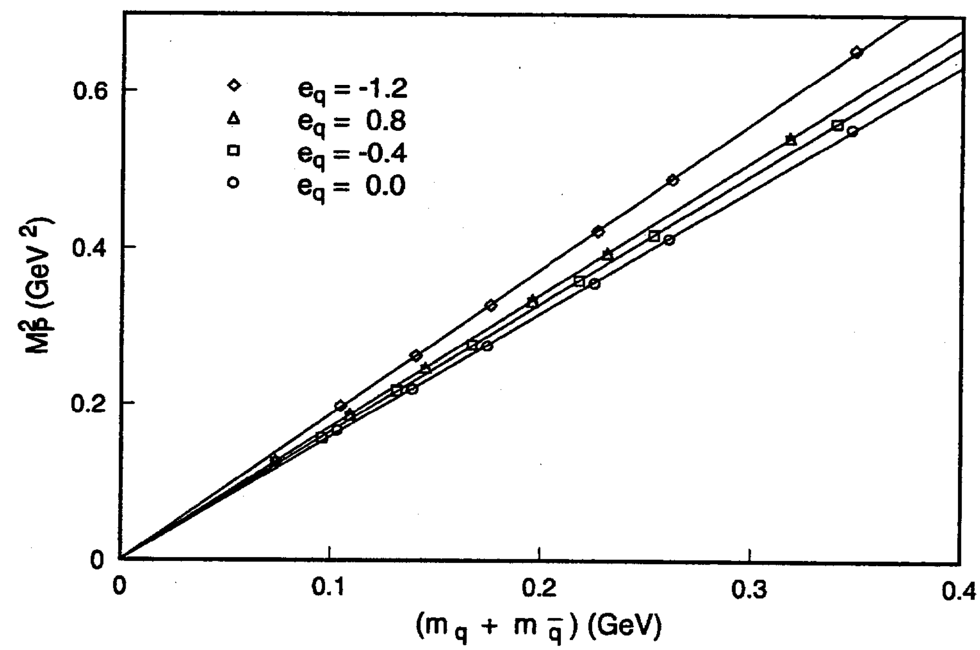

Figure 1: The mass squared, M_P^2, (in GeV^2) for neutral pseudoscalar meson versus lattice bare quark masses $m_q + m_{\bar{q}}$ (in GeV) is shown for various quark charges $e_q = 0.0, -0.4, 0.8$ and -1.2.

data.) The coefficient B in (1) which parametrizes the slope of m_P^2 may also be expanded in perturbation theory. Of the five possible e^4 terms in $B^{(2)}(e_q, e_{\bar{q}})$, only the $e_q^4, e_q^3 e_{\bar{q}}$ and $e_q^2 e_{\bar{q}}^2$ terms were found to improve the χ^2. The coefficients in A and B, along with the four values of κ_c for the four quark charges, constitute a 12-parameter fit to the meson mass values.

Before discussing the numerical results, we briefly describe the formulation of lattice QED which we have employed in these calculations. The gauge group in this case is abelian, and one has the choice of either a compact or noncompact formulation for the abelian gauge action. Lattice gauge invariance still requires a compact gauge-fermion coupling, but we are at liberty to employ a noncompact form of the pure photon action $S_{\rm em}$. Then the theory is free in the absence of fermions, and is always in the nonconfining, massless phase. An important aspect of a noncompact formalism is the necessity for a gauge choice. We use QCD lattice configurations which have all been converted to Coulomb gauge for previous studies of heavy-light mesons. Coulomb gauge turns out to be both practically and conceptually convenient in the QED sector as well.

For the electromagnetic action, we take

$$S_{\rm em} = \frac{1}{4e^2}\sum_{n\mu\nu}(\nabla_\mu A_{n\nu} - \nabla_\nu A_{n\mu})^2 \tag{2}$$

with e the bare electric coupling, n specifies a lattice site, ∇_μ the discrete lattice right-gradient in the μ direction and $A_{n\mu}$ takes on values between $-\infty$ and $+\infty$. Electromagnetic configurations were generated using (2) as a Boltzmann weight, subject to the linear Coulomb constraint

$$\bar{\nabla}_i A_{ni} = 0 \tag{3}$$

with $\bar{\nabla}$ a lattice left-gradient operator. The action is Gaussian-distributed so it is a trivial matter to generate a completely independent set in momentum space, recovering the real space Coulomb-gauge configuration by Fast Fourier transform. We fixed the global gauge freedom remaining after the condition (3) is imposed by setting the $p = 0$ mode equal to zero for the transverse modes, and the $\vec{p} = 0$ mode to zero for the Coulomb modes on each time-slice. (This implies a specific treatment of finite volume effects which will be discussed below). The resulting Coulomb gauge field $A_{n\mu}$ is then promoted to a compact link variable $U_{n\mu}^{\rm em} = e^{\pm iqA_{n\mu}}$ coupled to the quark field in order to describe a quark of electric charge $\pm qe$. Quark propagators are then computed for propagation through the combined SU(3)$\times$U(1) gauge field.

Table 1: Calculated shift of critical mass, Δm_c versus tadpole estimate for neutral pseudoscalar mesons with various quark charges, e_q. All masses are in lattice units.

e_q	κ_c	δm_c	$\sum$ tadpole
0.0	0.16923(3)	—	—
-0.4	0.17130(2)	0.289(5)	0.251
0.8	0.17763(3)	1.118(5)	0.942
-1.2	0.18541(4)	2.063(6)	1.912

Next we discuss the evaluation of critical hopping parameters for nonzero quark charge. The self energy shift induced by electromagnetic tadpole graphs may be computed perturbatively. The one-loop tadpole graph is (for Wilson parameter r=1 and at zero momentum in Coulomb gauge)

$$\delta m_{EM} = \frac{e^2}{L^4}\sum_{k\neq 0}\{\frac{1}{4\sum_\mu \hat{k}_\mu^2} + \frac{1}{8\sum_i \hat{k}_i^2}\} \tag{4}$$

where k_μ are the discrete lattice momentum components for a L^4 lattice and $\hat{k}_\mu = \sin(k_\mu/2)$. This is entirely analogous to the well known QCD term δm_{QCD} [8]. The mass shift is then given by the sum over multiple insertions at the same point, which exponentiates the one-loop graph. The usual strong QCD corrections at $\beta = 5.7$ are given in this approximation by an overall multiplicative factor of $1/(8\kappa_c^{e=0})$. Together this produces a shift of the critical inverse hopping parameter of

$$\Delta m_c \equiv \left(\frac{1}{2\kappa_c} - \frac{1}{2\kappa_c^{e=0}}\right) = \frac{1}{8\kappa_c^{e=0}}(1 - e^{-\delta m_{EM}}) \tag{5}$$

The contribution from the conventional one loop radiative correction graph is found to be about one third the size of the tadpole. In Table 1, our numerical results for κ_c and the associated Δm_c is compared with the results using only the perturbative tadpole resummed result for the EM interactions(5).

For charge zero quarks, propagators were calculated at hopping parameter 0.161, 0.165, and 0.1667, corresponding to bare quark masses of 175, 83, and 53 MeV respectively. The gauge configurations are generated at $\beta = 5.7$, and we have taken the lattice spacing to be $a^{-1} = 1.15$ GeV as determined in Ref. [9]. After shifting by the improved perturbative values listed in Table 1, we select the same three hopping parameters for the nonzero charge quarks.

Because this shift turns out to be very close to the observed shift of κ_c, the quark masses for nonzero charge are nearly the same as those for zero charge. For all charge combinations, meson masses were extracted by a two-exponential fit to the pseudoscalar propagator over the time range $t = 3$ to 11. Smeared as well as local quark propagator sources were used to improve the accuracy of the ground state mesons masses extracted. Errors on each mass value are obtained by a single-elimination jackknife. The resulting data is fitted to the chiral/QED perturbative formula (1) by χ^2 minimization. The fitted parameters are given in Table 2. Errors were obtained by performing the fit on each jackknifed subensemble.

Aside from very small corrections of order $(m_d - m_u)^2$, the $\pi^+ - \pi^0$ mass splitting is of purely electromagnetic origin, and thus should be directly calculable by our method. Because we have used the quenched approximation, $u\bar{u}$ and $d\bar{d}$ mesons do not mix. The neutral pion mass is obtained by averaging the squared masses of the $u\bar{u}$ and $d\bar{d}$ states. (In full QCD the $u\bar{u}$ and $d\bar{d}$ mix in such a way that the neutral octet state remains a Goldstone boson of approximate chiral SU(3)×SU(3). By averaging the squared masses of $u\bar{u}$ and $d\bar{d}$ in the quenched calculation, we respect the chiral symmetry expected from the full theory. By contrast, linear averaging of the masses would give a π^0 mass squared nonanalytic in the quark masses). Thus, to zeroth order in e^2, the terms proportional to quark mass [2] cancel in the difference $m_{\pi^+}^2 - m_{\pi^0}^2$. This difference is then given quite accurately by the single term

$$m_{\pi^+}^2 - m_{\pi^0}^2 \approx A^{(1)} e^2 \tag{6}$$

Using the coefficients listed in Table 2, and the experimental values of the π^0, K^0, and K^+ masses, we may directly solve the resulting three equations for the up, down, and strange masses. The $\pi^+ - \pi^0$ splitting may then be calculated, including the very small contributions from the order $e^2 m_q$ terms. We obtain

$$m_{\pi^+} - m_{\pi^0} = 4.9 \pm 0.3\text{MeV} \tag{7}$$

compared to the experimental value of 4.6 MeV. (The electromagnetic contribution to this splitting is estimated [10] to be 4.43 ± 0.03 MeV.) Our calculation can be compared to the value 4.4 MeV (for $\Lambda_{\text{QCD}} = 0.3$ GeV and $m_s = 120$ MeV) obtained by Bardeen, Bijnens and Gerard[11] using large N methods. The values obtained for the bare quark masses are

$$m_u = 3.86(3), \quad m_d = 7.54(5), \quad m_s = 147(1) \tag{8}$$

The errors quoted are statistical only, and are computed by a standard jackknife procedure. The *extremely* small statistical errors reflect the accuracy of the pseudoscalar mass determinations, and should facilitate the future study of systematic errors (primarily finite volume, continuum extrapolation[13] and quark loop effects), which are expected to be considerably larger. The relationship between lattice bare quark masses and the familiar current quark masses in the $\overline{MS}$ continuum regularization is perturbatively calculable[14].

The presence of massless, unconfined degrees of freedom implies that the finite volume effects in the presence of electromagnetism may be much larger than for pure QCD. In fact, the corrections are expected to fall as inverse powers of the lattice size, instead of exponentially. We have estimated the size of the finite volume correction phenomenologically by considering the discussion of Bardeen, et.al[11], which models the low-q^2 contribution to the $\pi^+ - \pi^0$ splitting in terms of π, ρ, and $A1$ intermediate states. This gives the splitting as an integral,

$$\delta m_\pi^2 = \frac{3e^2}{16\pi^2}\int_0^{M^2} \frac{m_A^2 m_\rho^2}{(q^2+m_\rho^2)(q^2+m_A^2)} dq^2 \tag{9}$$

If the upper limit M^2 is taken to infinity, this reproduces the result of Ref.[12], which gives $\delta m_\pi = 5.1 MeV$. Even better agreement with experiment is obtained by matching the low-q^2 behavior with the large-q^2 behavior from large N perturbative QCD[11]. Here we only use the expression to estimate the finite volume correction, for which the low-q^2 expression above should be adequate. To estimate the finite volume effect, we cast this expression as a four-dimensional integral over d^4q and then construct the finite volume version of it by replacing the integrals with discrete sums (excluding the $q = 0$ mode). For a $12^3 \times 24$ box with $a^{-1} = 1.15$ GeV, we find that the infinite volume value of 5.1 MeV is changed to $\delta m_\pi = 4.8$ MeV, indicating that the result we have obtained in our lattice calculation should be corrected upward by about 0.3 MeV, or about 6%. In further numerical studies, we will be able to determine the accuracy of this estimate directly by calculations on larger box sizes. A study of other systematics such as finite lattice spacing effects is also in progress, and will be reported in a subsequent publication.

For comparison with other results,[2, 3, 4] we quote the following mass ratios, which are independent of renormalization prescription,

$$\frac{m_d - m_u}{m_s} = .0249(3)\,, \quad \frac{m_u}{m_d} = .512(6) \tag{10}$$

With the errors shown, which are statistical only, these results differ significantly from

Table 2: Coefficients of fitting function, Eq.(1). Terms of order $e_q e_{\bar{q}}^3$ and $e_{\bar{q}}^4$ in $B^{(2)}$ and e^4 in A were consistent with zero and dropped from this fit. Numerical values are in GeV^2 and GeV for A and B terms respectively.

Parameter	Fit
A	$0.0143(10)(e_q + e_{\bar{q}})^2$
$B^{(0)}$	$1.594(11)$
$B^{(1)}$	$0.205(22)e_q^2 + 0.071(9)e_q e_{\bar{q}} + 0.050(7)e_{\bar{q}}^2$
$B^{(2)}$	$0.064(17)e_q^4 + 0.033(6)e_q^3 e_{\bar{q}} - 0.031(4)e_q^2 e_{\bar{q}}^2$

the lowest order estimate[2] which uses Dashen's theorem to estimate the electromagnetic contribution to the kaon splitting to zeroth order. This lowest order estimate neglects the quark mass dependence of the electromagnetic terms, which we have determined by our procedure. Specifically, the important corrections to the lowest order result come from terms involving the strange quark mass times the difference of up and down quark charges. These corrections are determined by the second and third terms in $B^{(1)}$ in Table 2. The Weinberg analysis predicts that the 4.0 MeV kaon splitting consists of 5.3 MeV from the up-down mass difference and -1.3 MeV from EM. In our results, the up-down mass difference contributes 5.9 MeV, with -1.9 MeV from EM. This goes in the direction indicated by the $\eta \to 3\pi$ decay rate [4], although our results do not deviate as much from the lowest order analysis as those of Ref. [4], where the quark mass contribution to the kaon splitting is estimated to be 7.0 MeV.

In the present work we have focused on the pseudoscalar meson masses. This is the most precise way of determining the quark masses as well as providing an important test of the method in the $\pi^+ - \pi^0$ splitting. Further calculations of electromagnetic splittings in the vector mesons and the baryons, as well as in heavy-light systems, are possible using the present method. This will provide an extensive opportunity to test the precision of the method and gain confidence in the results. Further study of electromagnetic properties of hadrons in lattice QCD, such as magnetic moments and form factors, is also anticipated.

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