Flavour Physics of Up, Down and Strange Quarks from Dynamical QCD $\times$ QED

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Lattice simulations of QCD are now reaching a precision, where isospin breaking effects can be investigated. These effects are caused by (i) mass differences between the up, down and strange quarks and (ii) electromagnetic effects due to the different charges of the quarks. So far most lattice QCD simulations are performed neglecting electromagnetic effects. In order to compute physical observables to high precision, it is important to include and control contributions from QED. In previous work we have outlined a program to systematically investigate the pattern of flavour symmetry breaking. The program has been successfully applied to meson and baryon masses involving up, down and strange quarks. In this project we extend the investigations to include matrix elements, charmed quarks and electromagnetic effects.

1 Introduction

One of the most profound open questions in particle physics is to understand the pattern of isospin and flavour symmetry breaking and mixing. Lattice simulations are now reaching a precision, where these effects can be investigated. They are due to two causes:

- The mass differences between the up, down and strange quarks
- Electromagnetic effects due to the different charges of the up, down and strange quarks

Bietenholz *et al.*[1,2] have outlined a program to systematically investigate the pattern of flavour symmetry breaking. The program has been successfully applied to meson and baryon masses involving up, down and strange quarks. In this project we extend the investigations to include matrix elements, charm quarks, the u, d mass difference and electromagnetic effects.

A distinctive feature of our simulations is the way we tune the light and strange quark masses. We have our best theoretical understanding when all three quark flavours have the same mass, because we can use the full power of $\mathrm{SU}(3)$ flavour symmetry. Starting from the $\mathrm{SU}(3)$ symmetric point, our strategy is to keep the singlet quark mass

$$\bar{m} = (m_u + m_d + m_s)/3 \tag{1}$$

fixed at its physical value, while

$$\delta m_q \equiv m_q - \bar{m} \tag{2}$$

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is varied, with $\delta m_u + \delta m_d + \delta m_s = 0$. As we move from the symmetric point $m_u = m_d = m_s$ (where the pion mass is $\approx 411\,\mathrm{MeV}$) to the physical point along the path $\bar{m} = const$, the s quark becomes heavier, while the u and d quarks become lighter. These two effects tend to cancel in any flavour singlet quantity. The cancellation is perfect at the symmetric point, and we have found that it remains good down to the lightest points we have simulated so far[2]. (In contrast, the procedure followed by most other collaborations is to first tune the strange quark mass m_s to its physical value and then vary the up and down quark masses.) This procedure leads to highly constrained extrapolations and reduces the number of free parameters drastically.

The dependence of hadronic matrix elements on up, down and strange quark masses has been worked out group-theoretically to LO, see for example Cooke *et al.*[3], similarly to the case of hadron masses[2]. That leads again to highly constrained extrapolations for nonsinglet quantities. When confronted with numerical calculations, this provides us with invaluable information on the pattern of flavour symmetry breaking. Flavour symmetry breaking effects in electroweak matrix elements are a key issue in precision tests of the Standard Model. A strong feature of our approach is that along the entire trajectory $\bar{m} = const$ both kaon and hyperon $V - A$ transition form factors are expected to vary at most quadratically in δm_q[4,5]. While the kaon semileptonic decay is a standard approach to the determination of the CKM matrix element $|V_{us}|$, we now also investigating the alternative hyperon semileptonic decay approach.

So far most lattice QCD simulations are performed neglecting electromagnetic (EM) effects. In order to compute physical observables to high precision, it is important to include and control contributions from QED. We have initiated a similar program, as the symmetry of the electromagnetic current is similar to that of the mass matrix,

$$m_u + m_d + m_s = 3\,\bar{m} \quad \Longleftrightarrow \quad e_u + e_d + e_s = 0\,. \tag{3}$$

In this project we use this expansion and complement our previous simulations by a fully dynamical simulation of QCD $\times$ QED.

We employ clover fermions with $N_f = 2 + 1$ flavours of dynamical quarks[6]. Clover fermions have exact flavour symmetry, and are nonperturbatively $O(a)$ improved (we have determined the improvement coefficient c_{sw} using the Schrödinger functional formalism). In our combined QCD $\times$ QED simulations the action is supplemented by a noncompact $U(1)$ gauge field[7], and the lattice Dirac operator becomes

$$\not{D}q(x) = \frac{1}{2a}\left[\gamma_\mu e^{-ie_q A_\mu(x)} U_\mu(x)\, q(x+\hat{\mu}) - \gamma_\mu e^{ie_q A_\mu(x)} U_\mu^\dagger(x-\hat{\mu})\, q(x-\hat{\mu})\right]. \tag{4}$$

We choose the electromagnetic coupling large enough so as to achieve a significant effect on hadron masses and matrix elements. The result will then be interpolated to the physical fine structure constant.

2 QCD

Let us first consider the case of pure QCD and highlight some of the salient features of our approach, along with a selection of results. We have space for hadron masses and the pattern of flavour symmetry breaking only.

With clover fermions the quark masses are defined by the distance from κ_c, the critical value of the hopping parameter κ. The bare quark masses then read

$$am_q = \frac{1}{2\kappa_q} - \frac{1}{2\kappa_c}\,, \tag{5}$$

where vanishing of the quark mass along the $\mathrm{SU}(3)$ flavour symmetric line determines κ_c.

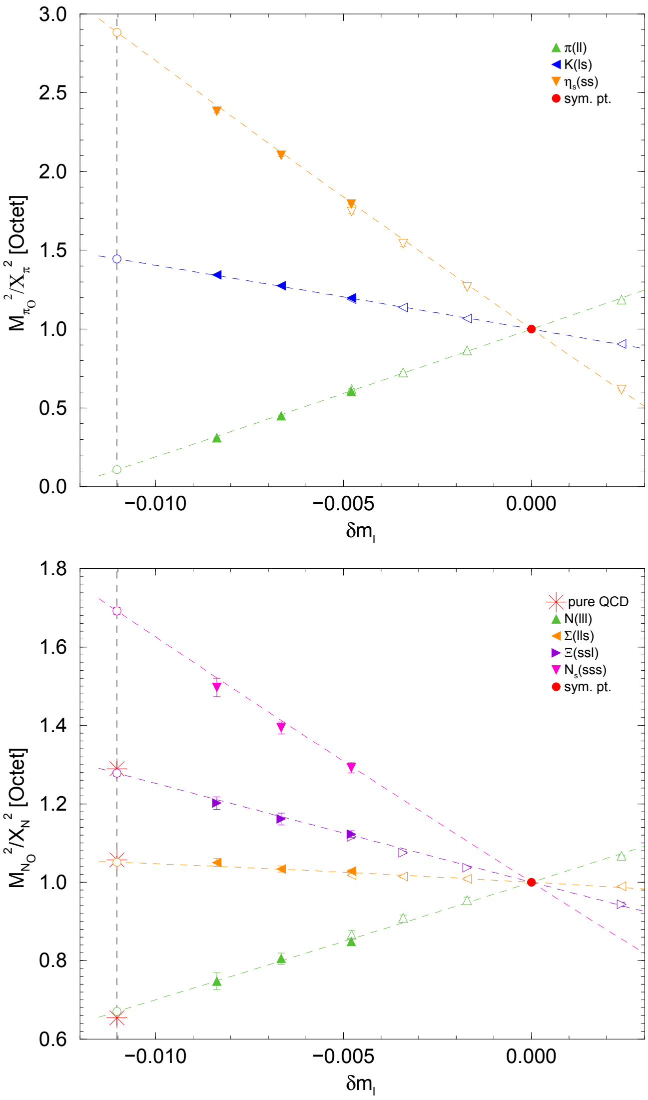

Figure 1. Top: the pseudoscalar meson octet "fan" plot of $M_{\pi_O}^2/X_\pi^2$ for $\pi_O = \pi, K, \eta_s$) versus δm_l. Bottom: the baryon octet "fan" plot of $M_{N_O}^2/X_N^2$ for $N_O = N, \Sigma, \Xi, N_s$) versus δm_l. Both sets of data are normalised to the singlet quantities $X_\pi^2 = (2M_K^2 + M_\pi^2)/3$ and $X_N^2 = (M_N^2 + M_\Sigma^2 + M_\Xi^2)/3$, respectively.

The initial value on this line, κ_0, is found by looking, for example, where $2m_K^2 + m_\pi^2$ is equal to its physical value.

Using symmetry arguments[2], we get the mass formula for the outer pseudoscalar mesons

$$\begin{aligned} M^2(a\bar{b}) = M_0^2 &+ \alpha\,(\delta m_a + \delta m_b) \\ &+ \beta_0\,(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + \beta_1\,(\delta m_a^2 + \delta m_b^2) + \beta_2\,(\delta m_a - \delta m_b)^2\,. \end{aligned} \tag{6}$$

For the outer octet baryons we obtain

$$\begin{aligned} M(aab) = M_0 &+ A\,(2\delta m_a + \delta m_b) \\ &+ B_0\,(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + B_1\,(2\delta m_a^2 + \delta m_b^2) + B_2\,(\delta m_a - \delta m_b)^2 \\ &+ B_3\,(\delta m_a^2 - \delta m_b^2)\,, \end{aligned} \tag{7}$$

and for the decuplet baryons we find

$$\begin{aligned} M(abc) = M_0 &+ A\,(\delta m_a + \delta m_b + \delta m_c) \\ &+ B_0\,(\delta m_u^2 + \delta m_d^2 + \delta m_s^2) + B_1\,(\delta m_a^2 + \delta m_b^2 + \delta m_c^2) \\ &+ B_2\,(\delta m_a^2 + \delta m_b^2 + \delta m_c^2 - \delta m_a\delta m_b - \delta m_a\delta m_c - \delta m_b\delta m_c)\,. \end{aligned} \tag{8}$$

In Fig. 1 we show the pseudoscalar octet and nucleon octet masses together with a combined fit, where the up and down quarks have been assumed mass degenerate,

$$m_u = m_d \equiv m_\ell\,. \tag{9}$$

In this case only one variable is needed to parameterise the symmetry breaking, as $\delta m_s = -2\delta m_\ell$. Typical 'fan' plots are seen with results radiating from the common SU(3) symmetric point. We also see an absence of any curvature in the data and the fits, predicting $\beta_0, \beta_1, \beta_2 \approx 0$ as well as $B_0, B_1, B_2, B_3 \approx 0$. This shows that the Gell-Mann–Okubo relations work all the way from the SU(3) symmetric to the physical point[2]. In Fig. 2 we show these results together with other recent results in a plot taken from Kronfeld[8], to which we refer to for more details.

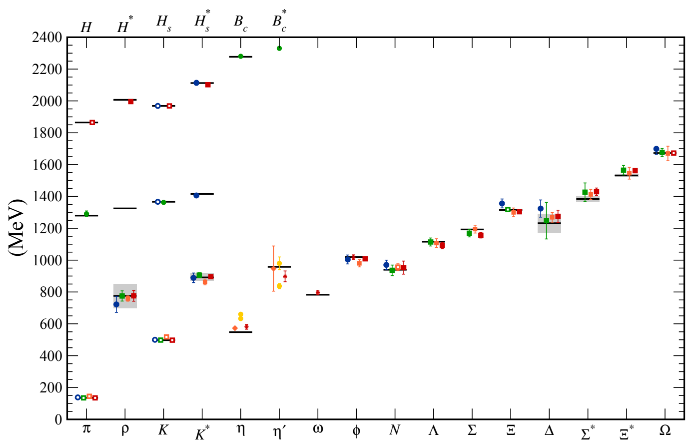

Figure 2. Results for the hadron masses at the physical point by various collaborations. Our points are the orange squares. The figure is taken from Kronfeld[8].

3 QCD × QED

In investigating the effects of SU(3) breaking due to quark mass differences, the group-theoretical analysis of the mass dependence[2] greatly helped us to organise our results. We now do the same with charge effects. We find in fact that the group theory for the two cases is very similar, and we can often simply read off the form of the electromagnetic effects from our quark mass results.

The symmetry of the electromagnetic current is similar to the symmetry of the quark mass matrix. The simplifications that we get in the mass case by imposing the constraint $m_u + m_d + m_s = const$ are similar to the simplifications that come from the identity $e_u + e_d + e_s = 0$, which reduces the number of allowed terms in the three-flavour case, when compared with two or four flavours. One difference between quark mass expansions and electromagnetic expansions is that in the mass expansion we can have both odd and even powers of δm_q, but in the expansion of hadron masses we are only allowed even powers of the quark charges. We can therefore read off the leading QED polynomials from Tab. 3 of Bietenholz *et al.*[2]. This should be all we need for simulations at the symmetric point. Away from the symmetric point we might want to consider mixed polynomials of the order $e_q^2 \delta m_q$, so that we can describe (for example) differences in the electromagnetic mass between the proton (uud) and the Σ^+ (uus), or between neutron (udd) and Ξ^0 (uss).

We can use symmetry arguments, just like those of Sec. 4 of Bietenholz *et al.*[2], to write down the leading order electromagnetic contributions M_{EM} to the masses of the outer octet mesons and nucleons and the decuplet baryons. We just drop the linear terms, and keep the quadratic terms, and change masses to charges. For the outer mesons we have

$$\begin{aligned} M^2_{EM}(a\bar{b}) &= \beta_0^{EM}(e_u^2 + e_d^2 + e_s^2) + \beta_1^{EM}(e_a^2 + e_b^2) + \beta_2^{EM}(e_a - e_b)^2 \\ &= \beta_0^{EM}(e_u^2 + e_d^2 + e_s^2) + (\beta_1^{EM} + \beta_2^{EM})(e_a^2 + e_b^2) - 2\beta_2^{EM} e_a e_b \,. \end{aligned} \tag{10}$$

The bottom form of the mass equation can be directly matched up with different classes of Feynman diagrams shown in Fig. 3. The first set of diagrams, with both ends of the photon line attached to the same valence quark (Fig. 3a), contributes to $(\beta_1^{EM} + \beta_2^{EM})$. The second set of diagrams, with the photon crossing between the valence lines (Fig. 3b), only contributes to β_2^{EM}. The final set of diagrams, with the photon attached to a sea quark bubble (Fig. 3c), only contributes to β_0^{EM}. This last set of diagrams would be missed out if the electromagnetic field was quenched instead of dynamical.

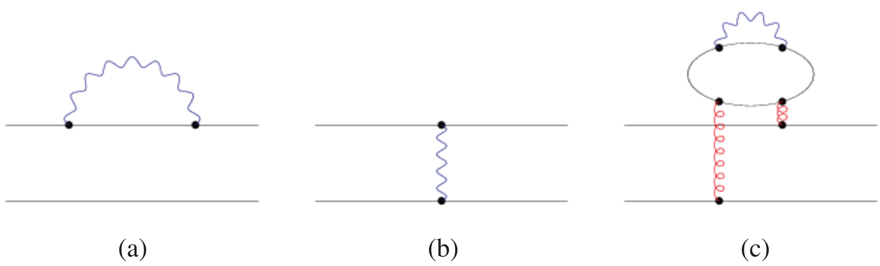

Figure 3. Examples of Feynman diagrams contributing to the meson electromagnetic mass.

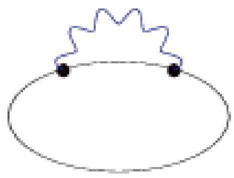

Figure 4. Example of a Feynman diagram contributing to the vacuum.

Our first dynamical QCD $\times$ QED run was made with $\kappa_u = \kappa_d = \kappa_s$, the same κ values we used for the symmetric point in pure QCD, and $e^2 = 1.25$. Our strategy is to simulate at an artificially large coupling, $\alpha_{\rm EM} \approx 1/10$, and then interpolate between this point and pure QCD to the physical value. The first point to mention is that diagrams like the one shown in Fig. 4 have a big effect on the QCD $\times$ QED vacuum. In Fig. 5 we show the effect on the average plaquette.

When QED is added the meson masses become much heavier, especially the $u\bar{u}$. We attribute this to a shift in κ_c for the quarks due to their electromagnetic self-interaction. (κ_c works rather like an additive renormalisation of the quark masses.) The up quark turns out to be considerably heavier than the two other, which is to be expected, because it has a larger charge. So, to keep the quark masses the same, we will need to simulate at a different set of κ values than those used in pure QCD.

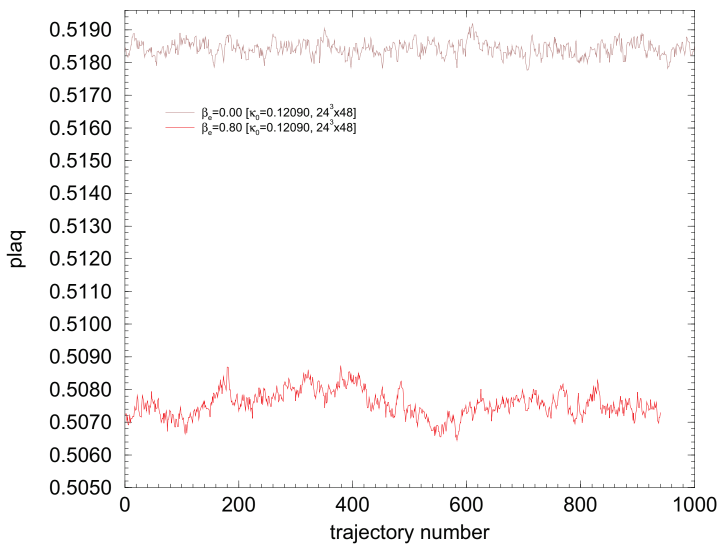

Figure 5. The average plaquette for pure QCD (top) and QCD $\times$ QED (bottom).

However, even with the present large quark masses we can already see some physical effects of QED, beyond this shift in κ_c. Extrapolated to the physical value of the fine structure constant, $\alpha_{EM} = 1/137$, our present data give

$$
\begin{aligned}
\beta_0^{EM} &= 0.034 \,, \\
\beta_1^{EM} &= 0.076 \,, \\
\beta_2^{EM} &= 0.031 \,.
\end{aligned}
\tag{11}
$$

β_0^{EM} receives contributions from quark-line disconnected diagrams, like that shown in Fig. 3c. It turns out that this contribution alone accounts for $\approx 2\%$ of the mass of the pseudoscalar mesons. From PCAC and/or the leading flavour expansion we expect that $M^2_{a\bar{b}} = (M^2_{a\bar{a}} + M^2_{b\bar{b}})/2$. Violations of this relation are 27-plet and cannot be present at leading order in the quark mass. Using Eq. 10, we see that the β_0^{EM} and β_1^{EM} terms cancel and the only term which contributes is β_2^{EM}, $M^2_{u\bar{d}} - (M^2_{u\bar{u}} + M^2_{d\bar{d}})/2 = \beta_2^{EM}$. The sign of β_2^{EM} is sensible. Opposite charges attract, like charges repel. So we would expect electromagnetic effects to raise the energy of the $u\bar{d}$ (π^+) meson (with a repulsive electromagnetic force between the valence quarks) relative to the $u\bar{u}$ and $d\bar{d}$ mesons (with attractive electromagnetic force between the valence quarks), and that is exactly what we find.

There is another difference between the up quark and the other two. The Z_m renormalisation factor will now depend on both the QCD coupling and the QED coupling, and the up quark will have a different Z_m, and a different anomalous dimension γ_m, from the other two quarks. This means that the ratio m_u/m_d now depends on renormalisation scheme and scale (even in the continuum). Likewise, isospin violating mass splittings, for example $M_n - M_p$, are scheme independent, but the question of how much of the splitting is due to the quark mass difference $m_d - m_u$, and how much is due to electromagnetic effects, becomes dependent on scheme and scale. This effect might be minor with $\alpha_{EM} \approx 1/137$, but might be more relevant with $\alpha_{EM} \approx 1/10$.

In pure QCD we can impose perfect $\mathrm{SU}(3)$ symmetry simply by making all three κ values equal. With QED present, there is no way to have perfect $\mathrm{SU}(3)$ symmetry, and so no completely unique way to define a line, where all three quark masses are equal. In particular, we cannot tune the κ values to make all members of an $\mathrm{SU}(3)$ multiplet degenerate. However, a physically reasonable definition is to look for the line, where the following neutral pseudoscalar meson masses are equal: $s\bar{d}$, $d\bar{s}$ (real particles) and $d\bar{d}$, $s\bar{s}$, $u\bar{u}$ (partially quenched mesons, with annihilation diagrams switched off, so that they do not mix with each other). This line will have $\kappa_s = \kappa_d \neq \kappa_u$.

This symmetric line will end at a point, where all the neutral pseudoscalar mesons are massless. We define this to be the chiral point, the point where all our quark masses are zero. In the case of the down and strange quark masses it is clear that this is the correct definition. Even with QED present, there is a chiral $\mathrm{SU}(2)$ symmetry connecting strange and down quarks. So, if both quarks are massless, there will be a massless Goldstone boson from the spontaneous symmetry breaking. Although the neutral mesons will be massless at the chiral point, the charged mesons can have a mass from electromagnetic effects, even when all the quark masses are zero. The charged axial currents are no longer conserved after QED is added to the action, so there is not a Goldstone theorem for the charged pseudoscalars.

Among the quantities we are currently looking at are the splittings of nucleon and kaon masses, as well as the kaon decay constant and the form factors of the semileptonic $K_{\ell 3}$ decay. Typically, the strong isospin violation and electromagnetic corrections are of the same order of magnitude. Of particular interest is the muon anomalous magnetic moment. It is one of the most precisely measured quantities in particle physics. Recent high precision measurements at Brookhaven Lab reveal a deviation of $\approx 3\sigma$ from the Standard Model, which could be a hint for new physics.

4 Outlook

Flavour symmetry and isospin breaking effects in hadron masses and matrix elements are among the most fundamental phenomena in particle physics. Within the Standard Model, they are described by essentially five parameters, the masses of up, down and strange quarks and the strength of the strong and electromagnetic interactions. It appears that these parameters need to be finely tuned to allow life. For example, a slight increase of the ratio m_d/m_u, and/or decrease of α_{EM}, would make the deuteron unstable and render nuclear fusion impossible. It is conceivable that some of the low-energy parameters of the Standard Model are uniquely determined by an underlying dynamical principle, similar to the prediction of the top quark mass[9]. Ultimately, that might be driven by an infrared fixed point of QCD $\times$ QED. (Indeed, a very recent calculation of the $\mathrm{SU}(3)$ beta function[10] suggests that QCD with two flavours of massless quarks has an infrared fixed point at $\alpha_{QCD} \approx 0.5$.) To shed light on this problem, and perhaps resolve the difference in mass between the up and down quark eventually, a first principles lattice calculation of QCD $\times$ QED is needed. Because hadrons are formed from bound states of quarks, there is no systematic way to treat electromagnetic effects in weak coupling perturbation theory.

Unfortunately, space limitations did not allow me to go into greater detail of this project and give full account of the present status of the calculations. But I am sure we will hear more about it at this Symposium.

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