Is the up-quark massless?

Hartmut Wittig

DESY

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Quark mass ratios in Chiral Perturbation Theory

- Leutwyler’s ellipse:

\[
\left( \frac{m_u}{m_d} \right)^2 + \frac{1}{Q^2} \left( \frac{m_s}{m_d} \right)^2 = 1
\]

\[(\text{Leutwyler, hep-ph/9609465})\]

\[
Q^2 = \frac{m_K^2}{m_\pi^2} \cdot \frac{m_K^2 - m_\pi^2}{(m_K^2 - m_{K^+}^2)_{\text{QCD}}}
\]

\[
\frac{m_K^2}{m_\pi^2} = \frac{m_s + \hat{m}}{m_u + m_d} \cdot \left\{ 1 + \Delta_M + O(m_s^2) \right\}
\]
• Results at next-to-leading order:

\[
\frac{m_u}{m_d} = 0.553 \pm 0.043, \quad \frac{m_s}{m_d} = 18.9 \pm 0.8
\]

Value of correction term \( \Delta M \) not known precisely...

• Cannot be estimated from phenomenology and chiral symmetry alone

• Large–\( N_c \) arguments and additional theoretical considerations suggest that \( \Delta M \) is small and positive (Leutwyler, hep-ph/9609465):

\[
0 < \Delta M < 0.13
\]

• However: magnitude and sign of \( \Delta M \) have not been derived from first principles

• If \( \Delta M \) were large and negative the up-quark could be massless

→ solution to the strong CP problem
The strong CP problem and $m_u = 0$

- QCD action with a $\theta$-term:

$$\theta \frac{g^2}{64\pi^2} \int d^4 x \ F \tilde{F}, \ 0 \leq \theta \leq 2\pi$$

- Induces CP violation in the strong sector, but no experimental evidence

- Value of $\theta$ is shifted by the quark mass matrix:

$$\bar{\theta} = \theta + \arg (\det M')$$

$\rightarrow$ explain why $\bar{\theta} \approx 0$

- If one of the quarks were massless one could perform a chiral $U(1)$ rotation with

$$-2N_f (\varphi_R - \varphi_L) = \arg (\det M')$$

which cancels the effects from $\theta$:

$$\Rightarrow \bar{\theta} = 0$$
• Require an approach to determine $\Delta_M$ based on first principles

• $\Delta_M$ is related to “low-energy constants” in the effective chiral Lagrangian

→ compute low-energy constants using lattice simulations of QCD

→ combine Chiral Perturbation Theory (ChPT) with Lattice QCD

Outline:

I. Basic concepts of Chiral Perturbation Theory

II. Strategy to compute low-energy constants

III. Results

IV. Summary
I. Basic concepts

• Effective chiral Lagrangian $\mathcal{L}_{\text{eff}}$

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{eff}}^{(2)} + \mathcal{L}_{\text{eff}}^{(4)} + \mathcal{L}_{\text{eff}}^{(6)} + \ldots$$

• Simultaneous expansion in powers of momentum $p$

and quark masses $m_u, m_d, m_s$

Order $p^2$:

$$\mathcal{L}_{\text{eff}}^{(2)} = \frac{F_0^2}{4} \text{Tr} \left( \partial_\mu U^\dagger \partial^\mu U \right) + \frac{F_0^2 B_0}{2} \text{Tr} \left( \mathcal{M}(U + U^\dagger) \right)$$

$$U = \exp \left( \frac{i T^a \varphi^a}{2 F_0} \right), \quad \mathcal{M} = \begin{pmatrix} m_u & m_d \\ m_d & m_s \end{pmatrix}$$

$F_0, B_0$: coupling ("low-energy") constants

→ Mathematical basis for “soft pion theorems” of the 1960’s

Order $p^4$:

...many more interaction terms...

coupling constants $L_1, L_2, \ldots, L_{10}, (L_{11}, L_{12})$
Loop corrections:

- One-loop corrections to $\mathcal{L}_{\text{eff}}^{(2)}$ generate logarithmic divergences, **but**

  form of counterterms **not** included in lowest order $\mathcal{L}_{\text{eff}}$

$\rightarrow$ Chiral Perturbation Theory (ChPT) is **non-renormalisable**

- Structure of $\mathcal{L}_{\text{eff}}$ determined by chiral symmetry:

  $\mathcal{L}_{\text{eff}}$ parameterised in terms of empirical constants $F_0, B_0, L_i$

$\rightarrow$ determine low-energy constants from phenomenology

**Examples:**

\[
L_1, L_2, L_3 : \quad \pi - \pi \text{ scattering}
\]

\[
L_5 : \quad \frac{F_K}{F_\pi} = 1 + \text{chiral log}'s + \frac{4(m_K^2 - m_\pi^2)}{F_\pi^2} L_5^r
\]

$\Rightarrow$ \[
L_5^r(m_\rho) = (1.4 \pm 0.5) \times 10^{-3}
\]
Need additional theoretical input to fix complete set of low-energy constants:

- Quark masses, $B_0$:

$$m^2_{\pi} = 2B_0\hat{m}, \quad m^2_K = B_0(m_s + \hat{m})$$
$$\hat{m} = \frac{1}{2}(m_u + m_d)$$

cannot determine $B_0$ or absolute magnitude of $\hat{m}$, $m_s$ without explicit knowledge of quark mass dependence

- Hidden symmetry in $L_{\text{eff}}$:

$$L_{\text{eff}} = L^{(2)}_{\text{eff}} + L^{(4)}_{\text{eff}}$$

invariant under

$$m_u \rightarrow m_u + \lambda m_d m_s \quad + \text{cyclic perm.}$$
$$L_{6,7} \rightarrow L_{6,7} + \frac{\lambda F_0^2}{32B_0}, \quad L_8 \rightarrow L_8 - \frac{\lambda F_0^2}{16B_0},$$

$\lambda$: arbitrary parameter

→ Chiral symmetry cannot distinguish between different sets $M^\lambda$, $L_{i}^\lambda$

“Kaplan-Manohar ambiguity” (1986)
Kaplan-Manohar ambiguity and \( m_u = 0 \)

- Leutwyler’s ellipse is mapped onto itself

- Expression for correction term \( \Delta_M \):

\[
\Delta_M = \frac{8(m_K^2 - m_\pi^2)}{F_\pi^2} (2L_8 - L_5) + \text{chiral log’s}
\]

- Experimental information on \( L_8 \) is afflicted with the KM ambiguity:

\[
\Delta_{GMO} = \frac{8(m_K^2 - m_\pi^2)}{F_\pi^2} (L_5 - 12L_7^\lambda - 6L_8^\lambda) + \text{log’s}
\]

- There is no direct experimental information on \( L_6, L_7, L_8 \) or \( \Delta_M \)

- QCD is not afflicted with KM ambiguity

**Test hypothesis** \( m_u = 0 \) **in lattice QCD:**

- Direct determination (difficult!)

- Compute quantities which provide information on \( L_8 \) or \( \Delta_M \) and are not subject to KM ambiguity

  → define effective chiral Lagrangian by determining the low-energy constants on the lattice from first principles
Use lattice simulations to

(1) Determine $L_i$ with high precision

$\rightarrow$ ChPT: analytic tool with numerically determined coupling constants
$\rightarrow$ test whether $m_u = 0$

(2) Determine $B_0$ and the absolute normalisation of quark masses;
combine with quark mass ratios obtained in ChPT

$\rightarrow m_s, m_d, m_u$

Aside: problem (2) has been solved in the "quenched approximation":

$$\frac{M_s}{\hat{M}} = 24.4 \pm 1.5, \quad \hat{M} = \frac{1}{2} (M_u + M_d)$$
(Leutwyler, Phys Lett B378 (1996) 313)

$$M_s + \hat{M} = 140 \pm 5 \text{ MeV}$$
(Garden, Heitger, Sommer, HW, Nucl Phys B571 (2000) 237)

$\Rightarrow M_s = 134 \pm 5 \text{ MeV}$

$$\overline{m}_{s}^{\text{MS}}(2 \text{ GeV}) = 97 \pm 4 \text{ MeV}$$
(all errors except quenching)
Lattice QCD:

- Quark masses are used as input parameters:

\[ m \rightarrow m_{PS}(m), F_{PS}(m) \]

→ Can map out the quark mass dependence of \( m_{PS} \) and \( F_{PS} \) without knowing the physical quark masses

↔ Phenomenology:

\[ m_\pi = m_{PS}(\hat{m}), \quad m_K = m_{PS}(\hat{m} + m_s) \]

- “partially quenched” QCD: can vary sea and valence quark masses independently

- Values of \( L_i \)'s depend only on \( N_f \)

→ Can determine their values even for unphysical quark masses
II. Strategy

ALPHA Coll. (Heitger, Sommer, HW), Nucl Phys B588 (2000) 377

- Modify and extend other proposals:

- Introduce reference quark mass $m_{\text{ref}}$ and define

$$R_F(x) = \frac{F_{\text{PS}}(m)}{F_{\text{PS}}(m_{\text{ref}})}$$

$$R_M(x) = \frac{\left(\frac{F_{\text{PS}}(m)}{G_{\text{PS}}(m)}\right)}{\left(\frac{F_{\text{PS}}(m_{\text{ref}})}{G_{\text{PS}}(m_{\text{ref}})}\right)} = \frac{\left(\frac{2m}{m_{\text{PS}}^2(m)}\right)}{\left(\frac{2m_{\text{ref}}}{m_{\text{PS}}^2(m_{\text{ref}})}\right)}$$

$$F_{\text{PS}}m_{\text{PS}} = \langle 0|A_0(0)|\text{PS}\rangle, \quad G_{\text{PS}} = \langle 0|P(0)|\text{PS}\rangle$$

$$m = xm_{\text{ref}}$$

$x$: dimensionless mass parameter

- $R_F, R_M$ are universal functions of $x$:
  Renormalisation factors drop out;
  straightforward extrapolation to the continuum limit

- Control over lattice artefacts: can isolate dynamical quark effects unambiguously

- Can compute $R_X(x)$ with high statistical precision
Expressions for $R_X$ in ChPT

• Consider QCD with $N_f = 3$ degenerate flavours (S. Sharpe 1997)

• Notation:

\[
y = \frac{2B_0 m}{(4\pi F_0)^2}, \quad x = \frac{y}{y_{\text{ref}}}, \quad \alpha_i = 8(4\pi)^2 L_i
\]

• Numerator $m^{\text{sea}} = m^{\text{val}} = m$; denominator: $m^{\text{sea}} = m^{\text{val}} = m_{\text{ref}}$

\[
R_M(x) = 1 - \frac{1}{3} \left[ x \ln x + (x - 1) \ln y_{\text{ref}} \right] - y_{\text{ref}}(x - 1) \left[ (2\alpha_8 - \alpha_5) + 3(2\alpha_6 - \alpha_4) \right]
\]

\[
R_F(x) = 1 - \frac{3}{2} \left[ x \ln x + (x - 1) \ln y_{\text{ref}} \right] + y_{\text{ref}}(x - 1) \frac{1}{2} (\alpha_5 + 3\alpha_4)
\]

• Numerator $m^{\text{val}} = m$, $m^{\text{sea}} = m_{\text{ref}}$; denominator: $m^{\text{sea}} = m^{\text{val}} = m_{\text{ref}}$

→ sensitive to different combinations of $\alpha_i$’s, e.g.

\[
R_F(x) = 1 - \frac{3}{4} \left[ (x + 1) \ln \left( \frac{1}{2}(x + 1) \right) + (x - 1) \ln y_{\text{ref}} \right] + y_{\text{ref}}(x - 1) \frac{1}{2} \alpha_5
\]

• Can determine $\alpha_4$, $\alpha_5$, $\alpha_6$ and $\alpha_8$
• Quenched approximation:

Additional parameters in $\mathcal{L}_{\text{eff}}^{(2)}$ associated with flavour-singlet field

$$R_M(x) = 1 - \frac{2}{3} \alpha_{\Phi} \left[ x \ln x + (x - 1) \left( \frac{1}{2} + \ln y_{\text{ref}} \right) \right]$$

$$+ \delta \ln x - y_{\text{ref}} (x - 1) \left( 2 \alpha_8^{(0)} - \alpha_5^{(0)} \right)$$

$$R_F(x) = 1 - y_{\text{ref}} (x - 1) \frac{1}{2} \alpha_5^{(0)}$$

• Estimates for $\delta$, $\alpha_{\Phi}$:

$$\delta \approx 0.10 - 0.14 \quad \text{(CP-PACS, hep-lat/9904012)}$$

$$\delta \approx 0.065 \pm 0.013 \quad \text{(FNAL, hep-lat/0007010)}$$

$$\alpha_{\Phi} \approx 0.6 \quad \text{(S. Sharpe, Lattice '96)}$$

Meson spectroscopy data by CP-PACS described well for

$$\delta = 0.12 \pm 0.02, \quad \alpha_{\Phi} = 0$$

or

$$\delta = 0.05 \pm 0.02, \quad \alpha_{\Phi} = 0.5$$

but not

$$\delta = 0.12 \pm 0.02, \quad \alpha_{\Phi} = 0.5$$
Extracting the low-energy constants from $R_X$

- Obtain $\alpha_i$ from least-$\chi^2$ fits to $R_X(x)$ over a suitably chosen interval in $x$.

- Alternatively, consider

\[ \Delta R_X(x_1, x_2) \equiv R_X(x_1) - R_X(x_2), \quad x_1 < x_2 \]

- Obtain $\alpha_i$ from simple algebraic expressions; vary $x_1, x_2$ to check stability

Example:

\[ \alpha_5^{(0)} = 2 \frac{\Delta R_{F}^{\text{quen}}(x_1, x_2)}{(x_1 - x_2) y_{\text{ref}}} \]
III. Results

• Test viability of the method:
  – statistical precision in continuum limit
  – stability in extraction of $\alpha_i$'s
  $\rightarrow$ use quenched approximation

• Numerical details:
  – 4 values of $a$: $a \approx 0.05 - 0.1 \text{ fm}$
    $L \approx 1.5 \text{ fm}$
  – $O(a)$ improved Wilson fermions
  – Reference point defined at
    \[
    (m_{PSr0})^2 = 3 \quad \Rightarrow \quad \begin{cases} 
    m_{\text{ref}} \approx m_s \\
    y_{\text{ref}} = 0.3398 \ldots \end{cases}
    \]
  – Interpolate $R_X$ to common values of
    \[
    x = 0.75, 0.80, \ldots, 1.40
    \]

• Observe stable continuum extrapolations
• \( R_M(x), R_F(x) \) in the continuum limit:

\[
R_M(x) = 1 + (x - 1)y_{\text{ref}}^{\frac{1}{2}}\alpha_5^{(0)}
\]

• Linearity of \( R_F(x) \) matched by expression in quenched ChPT, c.f.

• Several competing effects have to produce flat behaviour of \( R_M(x) \)

• Restrict \( x \)-interval to \( 0.75 \leq x \leq 0.95 \)
• Obtain very stable estimates for $\alpha_5^{(0)}$
  (independent of $\delta, \alpha_\Phi$)

$$\alpha_5^{(0)} = 0.989 \pm 0.064 \quad \text{(stat. error)}$$

- Insert estimates for $\delta$ and $\alpha_\Phi$ into expression for $R_M$;
determine $(2\alpha_8^{(0)} - \alpha_5^{(0)})$

$$(2\alpha_8^{(0)} - \alpha_5^{(0)}) = \begin{cases} 
0.35(5) & \delta = 0.12, \alpha_\Phi = 0 \\
0.02(5) & \delta = 0.05, \alpha_\Phi = 0.5 
\end{cases}$$
Stability analysis / Error estimates

• Higher orders in chiral expansion may modify estimates for \( \alpha_i \)'s.

\[ \rightarrow \text{systematic study requires data at smaller values of } x \]

• Estimate uncertainty due to higher orders; assume that

\[ O(x^2) \approx (O(x))^2, \quad O(x) \approx 0.20 \text{ at } x = 1 \]

alternatively, fit to

\[ R_F(x) = 1 + (x - 1)y_{ref} \frac{1}{2} \alpha_5^{(0)} + d_F y_{ref}^2 (x^2 - 1) \]

\[ 0.75 \leq x \leq 1.4 \]

\[ \rightarrow \text{uncertainty in } \alpha_5^{(0)}, (2\alpha_8^{(0)} - \alpha_5^{(0)}) \text{ amounts to } \pm 0.2. \]
QCD with $N_f = 2$

- Simulation with $N_f = 2$ degenerate flavours of dynamical quarks by UKQCD Collaboration;
  → identify with physical $u$ and $d$ quarks

- Numerical details:
  - only one value of $a$: $a \approx 0.1$ fm
    $L \approx 1.5$ fm
  → No control over continuum limit
  - sea quarks: $m_{PS}/m_V \approx 0.58$ (cf. $m_\pi/m_\rho = 0.169$)
  - $O(a)$ improved Wilson fermions
  - Reference point defined at

  $$(m_{PS}r_0)^2 = 2.092 \quad \Rightarrow \quad \begin{cases} m_{ref} \approx 0.7m_s \\ y_{ref} = 0.2370 \ldots \end{cases}$$

- Consider degenerate & non-degenerate combinations of valence quarks:

  $m_1^{val} = m_2^{val} = x m_{ref}, \quad m^{sea} = m_{ref}, \quad \text{“VV”}$
  $m_1^{val} = x m_{ref}, \quad m_2^{val} = m^{sea} = m_{ref}, \quad \text{“VS”}$
• Results for “VV” and “VS” cases

![Graphs showing comparisons between VV and VS cases with statistical and higher order uncertainties.]

• Consistency between “VV” and “VS” cases

• Uncertainties due lattice artefacts $\approx$ statistical error

• Uncertainties due to higher order orders $\approx \pm 0.2$
Results & Comparison

Renormalisation scale: $\mu = 4\pi F_\pi = 1175$ MeV

- Quenched ($N_f = 0$) Theory:

  $$\alpha_5^{(0)} = 0.99 \pm 0.06 \pm 0.2$$
  $$\alpha_8^{(0)} = \left\{ \begin{array}{ll}
  0.67 \pm 0.04 \pm 0.2, & \delta = 0.12, \alpha_\Phi = 0 \\
  0.50 \pm 0.04 \pm 0.2, & \delta = 0.05, \alpha_\Phi = 0.5
\end{array} \right.$$

- Partially quenched ($N_f = 2$) Theory

  $$\alpha_5^{(2)} = 1.22 \pm 0.13 \pm 0.25$$
  $$\alpha_8^{(2)} = 0.79 \pm 0.06 \pm 0.21$$

- Comparison with conventional ChPT:

  $$\alpha_5^{(3)} = 0.5 \pm 0.6, \quad \text{“standard”}$$
  $$\alpha_8^{(3)} = \left\{ \begin{array}{ll}
  0.76 \pm 0.4, & \text{“standard”} \\
  -0.9 \pm 0.4, & m_u = 0
\end{array} \right.$$
The value of $F_K/F_\pi$

- Experimental result $F_K/F_\pi = 1.22 \pm 0.01$ serves to determine $\alpha_5$

→ can use lattice estimates to predict $F_K/F_\pi$

→ check if results make sense phenomenologically

- Analyse lattice data for $N_f = 2$ “as if” they had been generated with $N_f = 3$

  $\alpha_5^{(3)} = 0.98 \pm 0.13 \pm 0.24$

  $\alpha_8^{(3)} = 0.59 \pm 0.06 \pm 0.21$

\[
\frac{F_K}{F_\pi} = 1 + \text{chiral log’s} + \frac{1}{2} \frac{m_K^2 - m_\pi^2}{(4\pi F_\pi)^2} \alpha_5^{(3)}
\]

\[
= 1.247 \pm 0.011 \pm 0.020
\]

→ suggests that quark mass dependence for $m \lesssim m_s$ is only weakly distorted by neglecting dynamical quarks.

- Compute mass correction $\Delta_M$:

\[
\Delta_M = \text{chiral log’s} + \frac{m_K^2 - m_\pi^2}{(4\pi F_\pi)^2} (2\alpha_8^{(3)} - \alpha_5^{(3)})
\]

\[
= -0.04 \pm 0.05 \pm 0.11
\]
Confront lattice results with the hypothesis $m_u = 0$:

\[ R_M(x) \]

\[ (2\alpha_8^{(3)}-\alpha_5^{(3)}) = 0.20^{+10}_{-12} \]

dashed line: expected behaviour if $m_u = 0$
IV. Summary

- Question whether $m_u = 0$ can be studied from first principles by combining Lattice QCD with Chiral Perturbation Theory:
  - Resolve ambiguity caused by hidden symmetry in $\mathcal{L}_\text{eff}$
  - Provide an absolute normalisation (e.g. $\hat{m} + m_s$)
    \[ \Rightarrow m_u, m_d, m_s \]

- Obtain accurate estimates for low-energy constants through ratios of matrix elements
  - conceptionally clean; good control over continuum limit
  - statistical precision of order $\pm 0.05$
  - uncertainties due to neglecting higher orders need to be investigated further
  - first results for $N_f = 0, 2$ do not support $m_u = 0$

- **Future:** require Monte Carlo data for $N_f = 3$ flavours of dynamical quarks
  - Algorithmic challenge: simulate odd $N_f$ efficiently for $m_{PS}/m_V < 0.5$
  - Statistical precision may be relaxed to study whether $m_u = 0$