Finite-volume effects and the electromagnetic contributions to kaon and pion masses

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Disentangling electromagnetic and isospin-violating effects in the pions and kaons is a long-standing issue.

Crucial for determining light-quark masses.

- Fundamental parameters in Standard Model; important for phenomenology.
- Size of EM contributions is the largest uncertainty in the determination of $m_u/m_d$.

<table>
<thead>
<tr>
<th></th>
<th>$m_u$ [GeV]</th>
<th>$m_d$ [GeV]</th>
<th>$m_u/m_d$</th>
</tr>
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<tr>
<td>value</td>
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<td>4.6</td>
<td>0.42</td>
</tr>
<tr>
<td>statistics</td>
<td>0.0</td>
<td>0.0</td>
<td>0.00</td>
</tr>
<tr>
<td>lattice</td>
<td>0.1</td>
<td>0.2</td>
<td>0.01</td>
</tr>
<tr>
<td>perturbative</td>
<td>0.1</td>
<td>0.2</td>
<td>--</td>
</tr>
<tr>
<td>EM</td>
<td>0.1</td>
<td>0.1</td>
<td>0.04</td>
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Reduce error by calculating EM effects on the lattice.
EM error in $m_u/m_d$ dominated by error in $(M_{K+}^2 - M_{K^0}^2)\gamma$, where $\gamma$ indicates the EM contribution.

Dashen (1960) showed that at leading order EM splittings are mass independent:

$$(M_{K+}^2 - M_{K^0}^2)\gamma = (M_{\pi^+}^2 - M_{\pi^0}^2)\gamma$$

Parameterize higher order effects ("corrections to Dashen’s theorem") by

$$(M_{K+}^2 - M_{K^0}^2)\gamma = (1 + \epsilon)(M_{\pi^+}^2 - M_{\pi^0}^2)\gamma$$

Note: $\epsilon$ is not exactly same as quantity defined by FLAG (Colangelo et al., arXiv: 1310.8555), which uses experimental pion splittings. But EM splitting should be $\approx$ experimental splitting, since isospin violations for pions are small. Using the experimental splitting gives an alternative result, which enters systematic error estimate.
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• Small volumes used only to test our understanding of finite-volume effects, not for final analysis.

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Finite-Volume Effects

- Difference between $20^3$ (□) and $28^3$ (×) ensembles at $a=0.12$ fm is small compared to what we expect from BMW [arXiv: 1201.2787], and RM123 [arXiv:1303.4896] results.

- We are not currently able to resolve the differences (consistent with zero).
  - Sign of the difference actually varies fairly randomly as quark masses change.

- Our recent work has been focused on understanding the (surprisingly small) FV effects in our data.
Hayakawa and Uno [arXiv:0804.2044] calculated the EM finite-volume effects in ChPT.

- Use noncompact realization of QED on the lattice, as we do.
- Found rather large effects.
- But noncompact QED in finite-volume is not uniquely defined:
  - It is necessary to drop some zero modes, but dropping others appears to be optional.
  - In Coulomb gauge, action for $A_0$ is: $\frac{1}{2} \int (\partial_i A_0)^2$.
    - For path integral to be convergent, need to drop $A_0$ modes for 3-momentum $\vec{k}=0$, any $k_0$.
  - Action for $A_i$ is: $\frac{1}{2} \int \left[ (\partial_0 A_i)^2 + (\partial_j A_i)^2 \right]$.
    - Here, only required to drop mode with 4-momentum $k_\mu=0$.
    - Hayakawa & Uno drop all $A_i$ modes with $\vec{k}=0$.
    - MILC keeps modes with $\vec{k}=0$, $k_0\neq0$.  

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\[ \left\langle A_0(k) A_0(-k) \right\rangle = \begin{cases} \frac{1}{k^2}, & \vec{k} \neq 0; \\ 0, & \vec{k} = 0. \end{cases} \]

\[ \left\langle A_i(k) A_j(-k) \right\rangle = \begin{cases} \frac{1}{k^2} \left( \delta_{ij} - \frac{k_i k_j}{k^2} \right), & \vec{k} \neq 0; \\ 0, & \vec{k} = 0. \end{cases} \]
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Hayakawa and Uno have an argument for dropping zero modes based on the problem of having a single electric charge on a torus, due to Gauss’s law.

- Gauss’s law comes from the equation of motion for $A_0$.
- Hayakawa & Uno and MILC drop the same modes for $A_0$ so Gauss’s law solution is the same for both.
- Difference is only for $\vec{k}=0$ modes for $A_i$. 
Staggered version of NLO SU(3) $\chi$PT [C.B. & Freeland, arXiv:1011.3994]:

\[
\Delta M_{xy,5}^2 = q_{xy}^2 \delta_{EM} - \frac{1}{16\pi^2} e^2 q_{xy}^2 M_{xy,5}^2 \left[ 3 \ln \left( \frac{M_{xy,5}^2}{\Lambda_{\chi}^2} \right) - 4 \right]
- \frac{2\delta_{EM}}{16\pi^2 f^2} \frac{1}{16} \sum_{\sigma, \xi} \left[ q_{x\sigma} q_{xy} M_{x\sigma,\xi}^2 \ln (M_{x\sigma,\xi}^2) - q_{y\sigma} q_{xy} M_{y\sigma,\xi}^2 \ln (M_{y\sigma,\xi}^2) \right]
+ c_1 q_{xy}^2 a^2 + c_2 q_{xy}^2 (2m_\ell + m_s) + c_3 (q_x^2 + q_y^2) (m_x + m_y) + c_4 q_{xy}^2 (m_x + m_y) + c_5 (q_x^2 m_x + q_y^2 m_y)
\]

- $x, y$ are the valence quarks.
- $q_x, q_y$ are quark charges; $q_{xy} = q_x - q_y$ is meson charge.
- $\delta_{EM}$ is the LO LEC; $\xi$ is the staggered taste.
- $\sigma$ runs over sea quarks ($m_u, m_d, m_s$, with $m_u = m_d = m_\ell$).
- Finite-volume corrections coming from the sunset and photon tadpole graphs are non-trivial.
  - (FV corrections to meson tadpole are known from standard ChPT and are quite small).
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$$+ c_1 q_{xy}^2 a^2 + c_2 q_{xy}^2 (2m_\ell + m_s) + c_3 (q_x^2 + q_y^2) (m_x + m_y) + c_4 q_{xy}^2 (m_x + m_y) + c_5 (q_x^2 m_x + q_y^2 m_y)$$
Need to add photon diagrams together in order for Coulomb-gauge finite-volume difference (FV -∞V) to be well-defined.

Can then perform brute force difference of FV sum (over $2\pi n_i/L$ and $2\pi n_0/T$) from ∞V integral.
Evaluation of FV difference

- Evaluate difference of sum and integral by VEGAS.
- Take VEGAS integrand as difference between $\infty V$ integrand, and its evaluation at weighted average of the 16 corners of the FV hypercube containing the point.
- Checked against Hayakawa-Uno result (written in terms of 1-d integral over special functions).
There is a difference in FV part of photon tadpole between Hayakawa-Unno (HU) and MILC when $\vec{k} = 0$:

- HU omits the $\vec{k} = 0$ piece entirely.
- For MILC, FV integrand is $\frac{3}{k^2} = \frac{3}{k_0^2}$, as long as $k_0 \neq 0$.
- Difference (MILC-HU) = $\frac{q^2}{L^3T} \sum_{n_0 \neq 0} \frac{3}{(2\pi n_0/T)^2} = \frac{q^2T}{4L^3}$.
- Our formulation has subtle $T, L$ dependence.
  - Fine if $L \to \infty$ first, or if both $T, L \to \infty$ with fixed ratio, but not if $T \to \infty$ first.
• Comparison of MILC and H-U FV corrections.
  ✦ An overall factor of $e^2 m^2$, (where $e$ and $m$ are charge & mass of the meson) has been taken out.

• $T/L$ values are the ones of our lattices.
  ✦ $T/L = 4.0, 5.33$ are the small lattices (~1.4 fm, ~1.8 fm) used only for investigating FV effects.

• H-U results are insensitive to $T$ in this range. (In their paper, they calculate in the $T=\infty$ limit only.)

• Our FV corrections are a factor of 2-3 less in most of the relevant range!
• ‘kaon’ and ‘pion’ points are the ones compared with BMW and RM123 results earlier.

• Each fit has 1 free parameter (overall height); shape is completely determined by ChPT at NLO.

• ChPT gives reasonable description of FV effects.

• Note that FV effect actually changes sign in ‘pion’ case.

• Can see why it is difficult to observe difference between results on $L=20$ and $L=28$ ensembles.
Mass-square difference between charge +1 mesons ($\pi^+$ & $K^+$) and ones made from uncharged valence quarks.

Shows unitary points only.

We have many partially quenched points, for charged and neutral mesons, as well as points with $2 \times$ physical charges.

~150 points in typical fit.

A big part the difference between results from different lattice spacings is from mis-tuned $m_s$, not discretization effects.
Points after correction for finite-volume effects.

Correction is ~7--10% (pions) and ~10--18% (kaons).

Bigger correction at higher mass because of overall factor of $m^2$ in 1-loop diagrams, but not at LO (Dashen’s theorem).

Note that $a \approx 0.12 \text{ fm}$, $m_l \approx 0.2m_s$ points for $L=20$ (□) and $L=28$ (×) are consistent.
Chiral fit to infinite-volume (corrected) points.

Data has very high correlations for different valence masses or charges on the same ensembles: covariance matrix nearly singular.

For that reason, and because errors are tiny (0.4--0.8%), it is difficult to get decent correlated fits.

This is a uncorrelated fit; has 149 data points, 29 parameters, $\chi^2/\text{dof}=127/120$, $p=0.34$ [uncorrel].

Fits are generally significantly better than earlier ones without FV corrections.
Chiral Fit and Extrapolation

\[ M_{xy}^2(q_x=2/3, q_y=-1/3) - M_{xy}^2(q=0) \]

- Extrapolate to continuum, and set valence, sea masses equal.
- Adjust \( m_s \) to physical value.
- Keep sea charges = 0.
- Small change between \( a=0.06 \) fm and continuum is conspiracy between discretization and \( m_s \) effects.

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Chiral Fit and Extrapolation

- Set sea quark charges to their physical values, using NLO chiral logs.

- Difference with previous case is very small for kaon; vanishes identically for pion.
• Neutral $\bar{d}d$-like mesons ($q_x = q_y = 1/3$) for same fit.

• Note difference in scale from charged meson plot.

• ~Function of $(m_x + m_y)$ only ($\pi$ and $K$ line up).

• Nearly linear: chiral logs vanish for neutrals.
Now subtract neutral masses from charged masses to give purple lines.

We are not including disconnected EM graphs for $\pi^0$, which is why we call it ‘$\pi^0$’.

Horizontal dotted line shows experimental value of $\pi$ splitting; difference between it and intercept of purple line with vertical, dashed-dotted physical $\pi$ line is a measure of systematic errors.

Can now read off ratio of $K$ and $\pi$ splittings:

$$\epsilon = 0.84(5)$$
Chiral Fit and Extrapolation

$M^2_{xy}(q_x=2/3, q_y=-1/3) - M^2_{xy}(q=0)$

- Alternative correlated fit, with data that has been thinned more.
- SVD-like cut is needed; we cut eigenvalues of correlation matrix that are < 1.
- 55 data points, 23 params, $\chi^2$/dof=53/32, p=0.01.
- Result is consistent with previous fit:

$$\epsilon = 0.79(8)$$
Systematic Errors

- Difference between the finite-volume corrected result for $\epsilon$ and the uncorrected one is 0.19. We currently take half this amount as the estimate of possible residual FV errors from higher orders in ChPT.

- Standard deviation on $\epsilon$ over all current continuum/chiral fits is 0.13.
  - Here we include all uncorrelated fits with $p > 10^{-3}$ or correlated fits with $p > 10^{-8}$.

- Instead of calculating $\epsilon$ by ratio of results for $K$ and $\pi$ splittings, we may use the experimental $\pi$ splitting. This gives $\epsilon = 1.02(4)$, or a difference from our central value of 0.18.
  - To be conservative, we take the larger number, 0.18, as an estimate of the lattice errors from the continuum/chiral extrapolation, although some of the difference may be due to residual finite-volume errors (included separately) or the effect of dropping disconnected diagrams for the $\pi^0$. 

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Get (preliminary!):

\[ \epsilon = 0.84(5)_{\text{stat}}(18)_{a^2}(10)_{\text{FV}} \]

or:

\[ \epsilon = 0.84(21) \]

Using this number with the current HISQ light meson analysis gives (preliminary!):

\[ m_u/m_d = 0.4482(48)_{\text{stat}}(^{+21}_{-15})_{a^2}(1)_{\text{FV}_{\text{QCD}}}(177)_{\text{EM}} \]

- where here “EM” denotes all errors from \( \epsilon \), while “FV_{\text{QCD}}” refers to finite-volume effects in the pure QCD calculation on the HISQ ensembles.
Future Plans

✧ We have data from additional ensembles at $a \approx 0.06$ fm and $a \approx 0.045$ fm.
  • need to complete analysis and add in to chiral/continuum extrapolation.

✧ EM effects in baryons also being studied.

✧ Extension to MILC HISQ ensembles is straightforward, and should reduce errors significantly:
  • Smaller discretization effects.
  • Nearly absent chiral extrapolation errors, since ensembles with physical masses are included.
  • Smaller FV effects, since our HISQ lattices are generally larger than the older asqtad ones. Max size $\sim 5.5$ fm.

✧ Extension to unquenched case will make possible controlled calculations of many additional quantities.
  • Dynamic (unquenched) QED code has been written, and has passed some basic tests.
• No evidence of any systematic problem in extracting masses in charged case (right) compared to uncharged case (left).

• BMW [arXiv:1406.4088] recently reported problems (close excited states) in extracting masses for the FV version of EM that we use, but in pure (quenched) QED.

• We see no such problems in our quenched QED + full QCD simulations. But agree that masses are $T$-dependent, as seen in the FV formulas.
In rest frame, \( p = (p_0,0,0,0) \), only the 00 component of the photon propagator contributes.

In infinite-volume, get:

\[
\int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \frac{(2p_0 + k_0)^2}{k^2 + m^2}
\]

where \( m \) is the meson mass, and denominator comes from momentum factors in the coupling of a \((\text{pseudo})\text{scalar}\) particle to a photon.
Finite-Volume ChPT: Sunset Graph

\[ \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2} \frac{(2p_0 + k_0)^2}{k^2 + m^2} \]

- \( k_0 \) integral, by itself, is linearly divergent.
- Even when we take difference between finite (spatial) volume version ["FV"] and infinite (spatial) volume version ["\( \infty V \)"], the \( k_0 \) integral makes the difference linearly divergent.
- (Usually, all divergences are the same in FV and \( \infty V \), so difference diagram by diagram is finite.)
- Problem here is coming from lack of Lorentz covariance of the gauge.
- But photon tadpole has a piece that cancels the spurious \( k_0 \) divergence.

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Finite-Volume ChPT: Photon Tadpole

- 00 piece of photon propagator gives:
- Combines with sunset to give:

\[- \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2}\]

\[\int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2} \left( \frac{(2p_0 + k_0)^2}{k^2 + m^2} - 1 \right)\]

- finite-volume effects of this integral (FV - ∞V) are now finite & calculable.
- Do by brute force difference of FV sum from ∞V integral.
  - FV sum over \(2\pi n_i / L\) for spatial directions; \(2\pi n_0 / T\) for time direction.

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Accidental very small FV difference between $20^3 \times 64$ (magenta) and $28^3 \times 64$ (black) lattices at RM123 comparison point.