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

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Motivation

- Disentangling electromagnetic and isospin-violating effects in the pions and kaons is long-standing issue.
- Crucial for determining light-quark masses.
  - Fundamental parameters in Standard Model; important for phenomenology.
  - Size of EM contributions is largest uncertainty in determination of m_u/m_d.

	m_u [GeV]	m_d [GeV]	m_u/m_d
value	1.9	4.6	0.42
statistics	0.0	0.0	0.00
lattice	0.1	0.2	0.01
perturbative	0.1	0.2	--
EM	0.1	0.1	0.04

MILC, arXiv:0903.3598

  - Reduce error by calculating EM effects on the lattice.

Background

- ✦ EM error in m_u/m_d dominated by error in $(M^2_{K^+} - M^2_{K^0})^\gamma$, where γ indicates the EM contribution.
- ✦ Dashen (1960) showed that at leading order EM splittings are mass independent:

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

- ✦ Parameterize higher order effects ("corrections to Dashen's theorem") by

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

  - Note: ϵ 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 ≈ experimental splitting, since isospin violations for pions are small. Using the experimental splitting gives an alternative result, which enters systematic error estimate.

Ensembles

- Table of ensembles used in the analysis:

$\approx a$[fm]	Volume	β	m_l/m_s	# configs.	L (fm)	$m_\pi L$
0.12	$12^3 \times 64$	6.76	0.01/0.05	1000	1.4	2.7
	$16^3 \times 64$	6.76	0.01/0.05	1003	1.8	3.6
	$20^3 \times 64$	6.76	0.01/0.05	2254	2.3	4.5
	$28^3 \times 64$	6.76	0.01/0.05	274	3.2	6.3
	$20^3 \times 64$	6.76	0.007/0.05	1261	2.3	3.8
	$24^3 \times 64$	6.76	0.005/0.05	2099	2.7	3.8
0.09	$28^3 \times 96$	7.09	0.0062/0.031	1930	2.3	4.1
	$40^3 \times 96$	7.08	0.0031/0.031	1015	3.3	4.2
0.06	$48^3 \times 144$	7.47	0.0036/0.018	670	2.8	4.5

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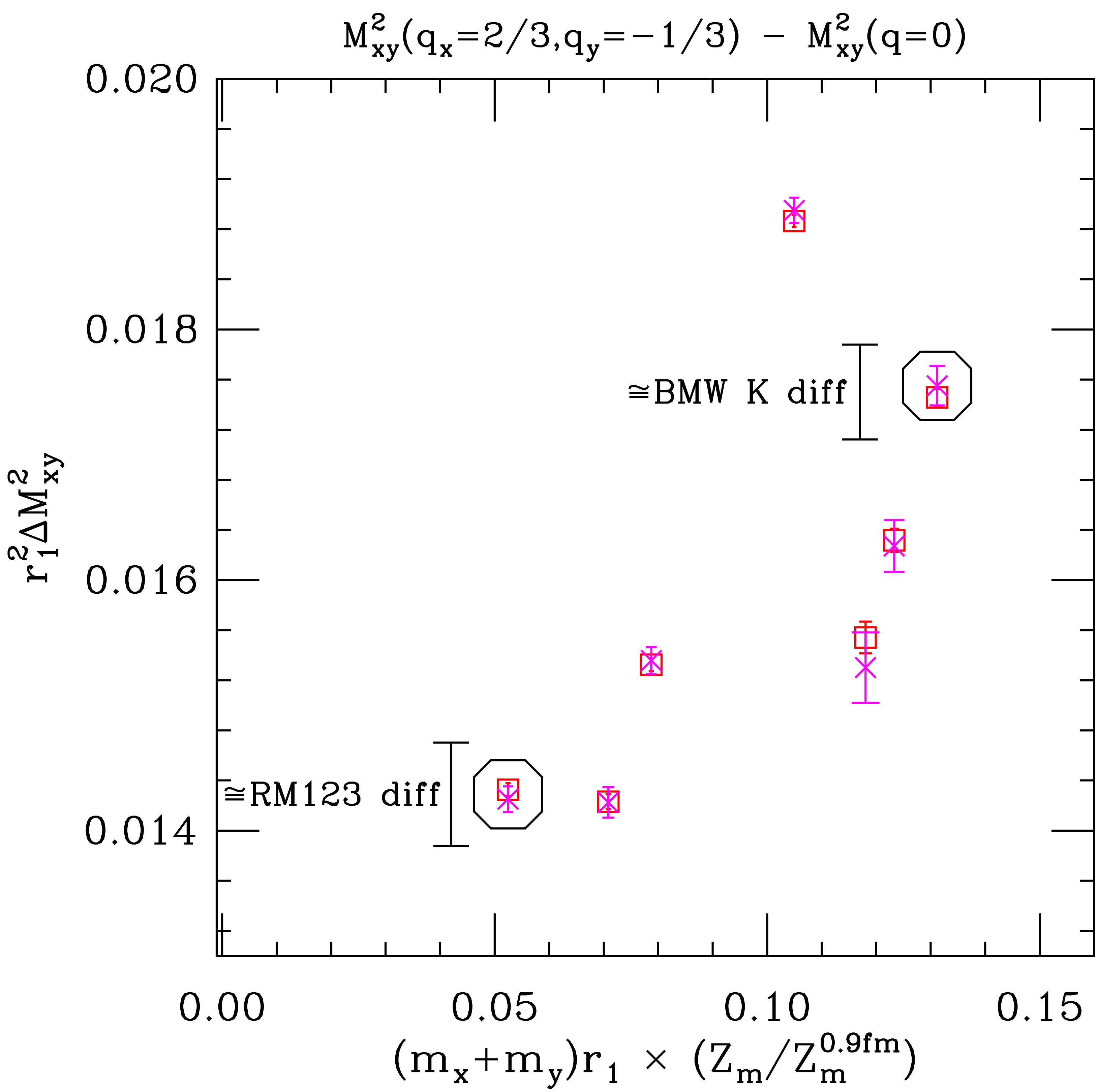
- From Bijnens and Daniellson [PRD 75, 104505 ('07)], quenched QED is sufficient for a controlled calculation of ϵ at NLO in SU(3) ChPT.

- Small volumes used only to test our understanding of finite-volume effects, not for final analysis.

Finite-Volume Effects



- Difference between 20^3 (□) and 28^3 (×) ensembles at $a \simeq 0.12$ 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.

Finite-Volume Effects in ChPT

- 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 $\vec{k}=0$, $k_0\neq 0$.

Finite-Volume Coulomb-Gauge Propagator

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

Hayakawa-Uno

$$\langle A_i(k)A_j(-k)\rangle = \begin{cases} \frac{1}{k^2}\left(\delta_{ij} - \frac{k_i k_j}{\vec{k}^2}\right), & \vec{k} \neq 0; \\ 0\ , & \vec{k} = 0. \end{cases}$$

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MILC

Finite-Volume Coulomb-Gauge Propagator

- 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.

Chiral Perturbation Theory

✦ Staggered version of NLO SU(3) χPT [C.B. & Freeland, arXiv:1011.3994]:

$$\Delta M^2_{xy,5} = q^2_{xy}\delta_{EM} - \frac{1}{16\pi^2}e^2 q^2_{xy} M^2_{xy,5}\left[3\ln(M^2_{xy,5}/\Lambda^2_\chi) - 4\right]$$
$$- \frac{2\delta_{EM}}{16\pi^2 f^2}\frac{1}{16}\sum_{\sigma,\xi}\left[q_{x\sigma}q_{xy}M^2_{x\sigma,\xi}\ln(M^2_{x\sigma,\xi}) - q_{y\sigma}q_{xy}M^2_{y\sigma,\xi}\ln(M^2_{y\sigma,\xi})\right]$$
$$+c_1 q^2_{xy}a^2 + c_2 q^2_{xy}(2m_\ell + m_s) + c_3(q^2_x + q^2_y)(m_x + m_y) + c_4 q^2_{xy}(m_x + m_y) + c_5(q^2_x m_x + q^2_y m_y)$$

- x,y are the valence quarks.
- q_x, q_y are quark charges; $q_{xy} \equiv q_x - q_y$ is meson charge.
- δ_{EM} is the LO LEC; ξ is the staggered taste
- σ runs over sea quarks (m_u, m_d, m_s, with $m_u = m_d \equiv m_\ell$)
- 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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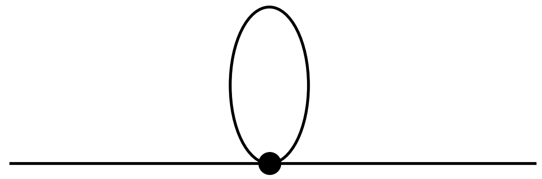

meson EM tadpole
(from short-distance
photons)

$$\begin{aligned}\Delta M^2_{xy,5} &= q^2_{xy}\delta_{EM} - \frac{1}{16\pi^2}e^2 q^2_{xy} M^2_{xy,5}\left[3\ln(M^2_{xy,5}/\Lambda^2_\chi) - 4\right] \\ &\quad - \frac{2\delta_{EM}}{16\pi^2 f^2}\frac{1}{16}\sum_{\sigma,\xi}\boxed{\left[q_{x\sigma}q_{xy}M^2_{x\sigma,\xi}\ln(M^2_{x\sigma,\xi}) - q_{y\sigma}q_{xy}M^2_{y\sigma,\xi}\ln(M^2_{y\sigma,\xi})\right]}\end{aligned}$$

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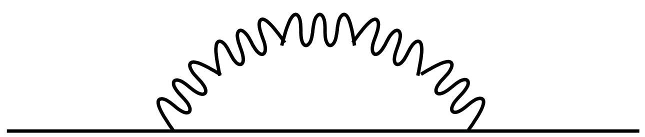
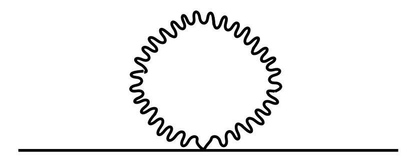
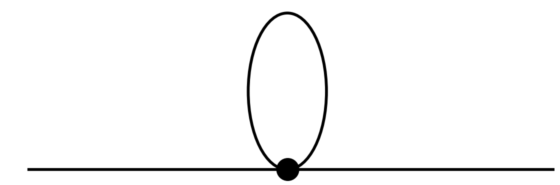
long-distance
photon contributions:



sunset



photon tadpole



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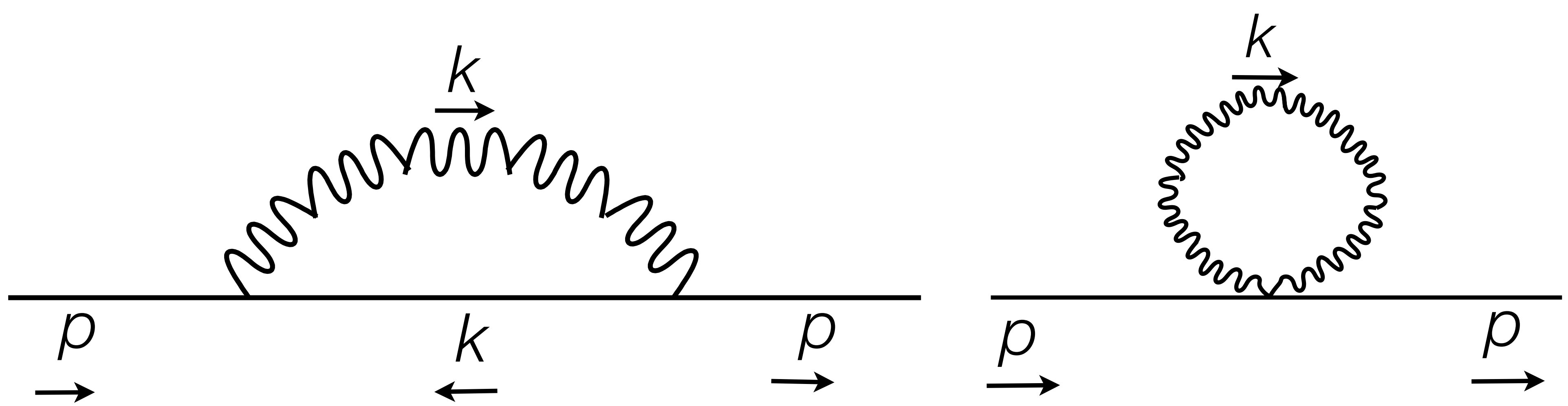
Finite-Volume ChPT

✦ Need to add photon diagrams together in order for Coulomb-gauge finite-volume difference (FV -∞V) to be well-defined.

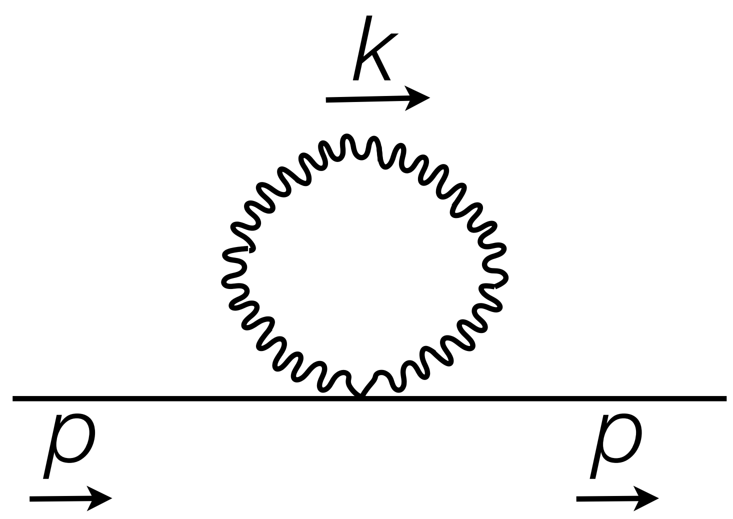


✦ Can then perform brute force difference of FV sum (over $2\pi n_i/L$ and $2\pi n_0/T$) from ∞V integral.

Evaluation of FV difference

- Evaluate difference of sum and integral by VEGAS.
- Take VEGAS integrand as difference between ∞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).

Photon Tadpole Graph

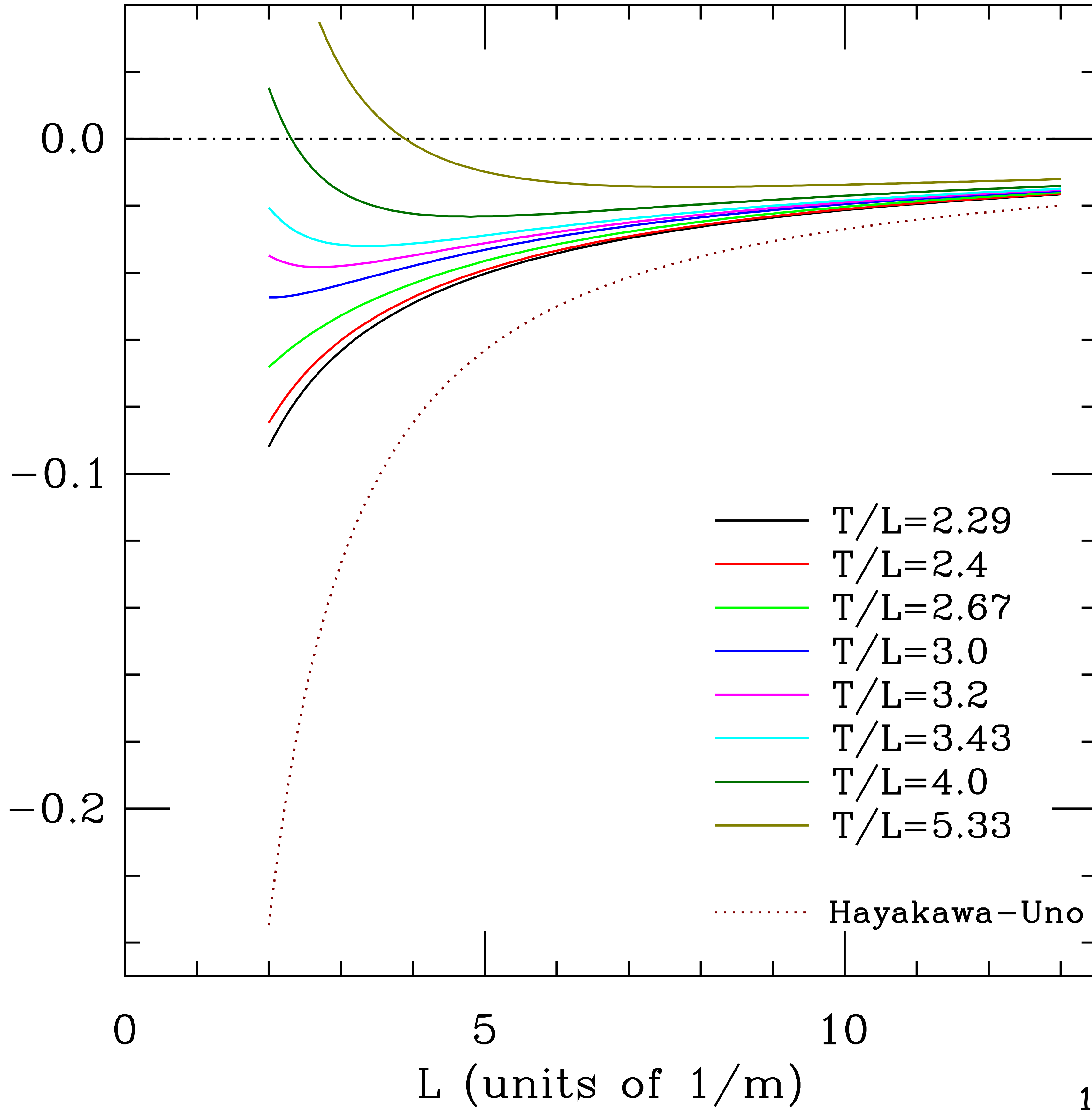


✦ There is a difference in FV part of photon tadpole between Hayakawa-Uno (HU) and MILC when $\vec{k} = 0$:

- 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) = $\dfrac{q^2}{L^3 T} \displaystyle\sum_{n_0 \neq 0} \dfrac{3}{(2\pi n_0/T)^2} = \dfrac{q^2 T}{4L^3}$.
- 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.

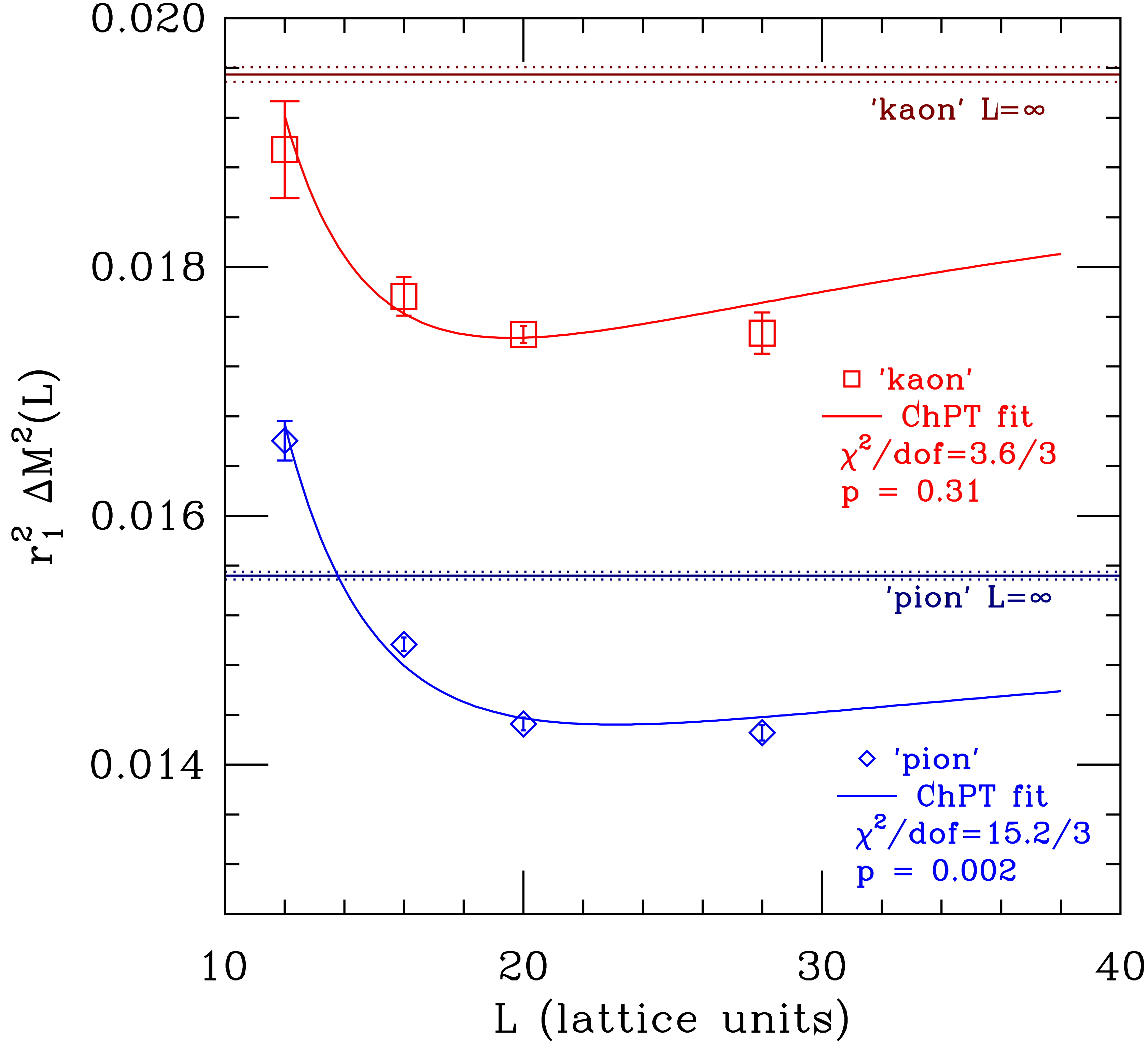
Finite-Volume Corrections

- 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!



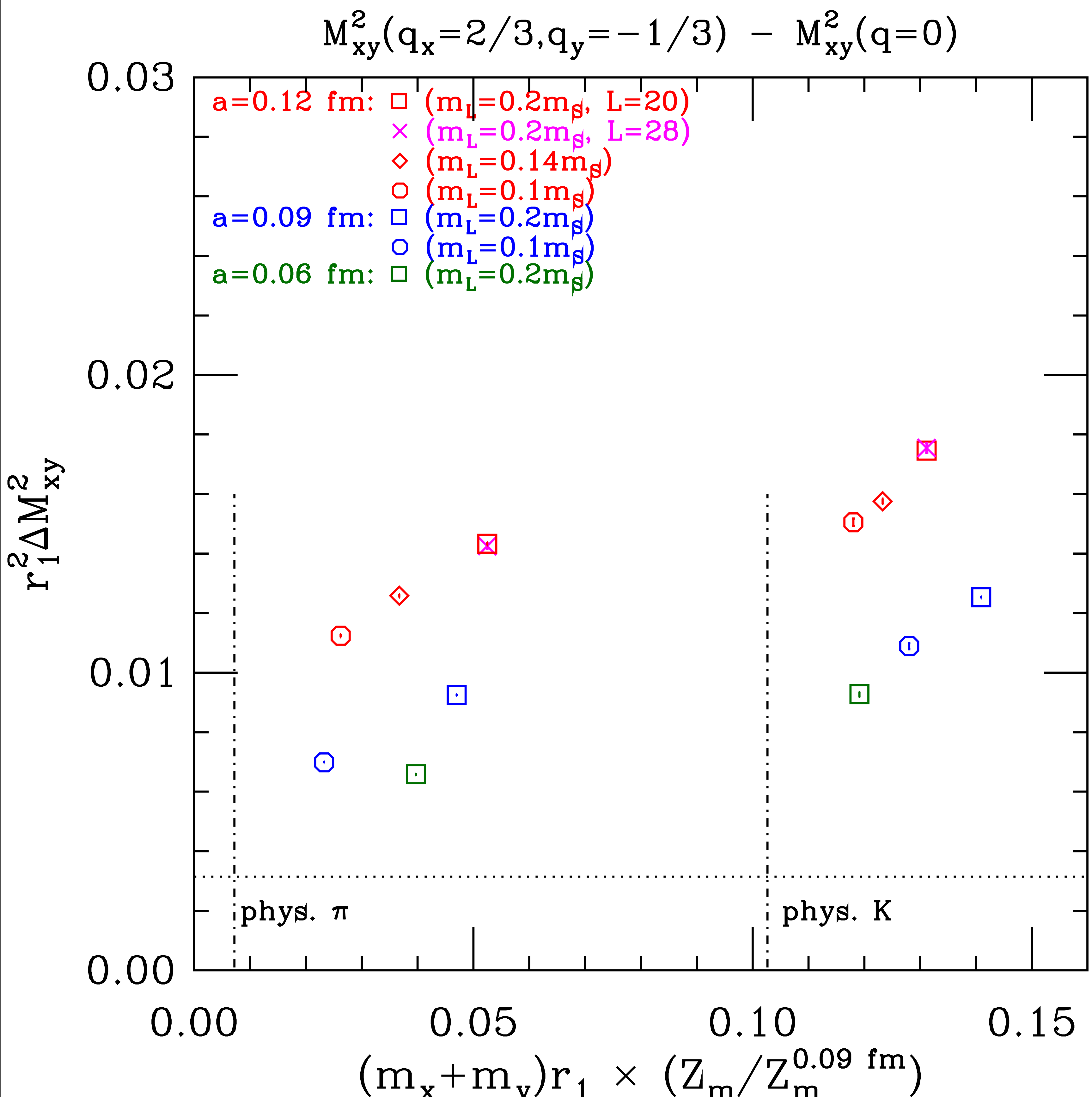
FV Corrections: Comparison with Data

- ‘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.



$a \simeq 0.12$ fm, $m_l/m_s = 0.01/.05$

Chiral Fit and Extrapolation



- Mass-square difference between charge +1 mesons (π^+ & 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 × 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.

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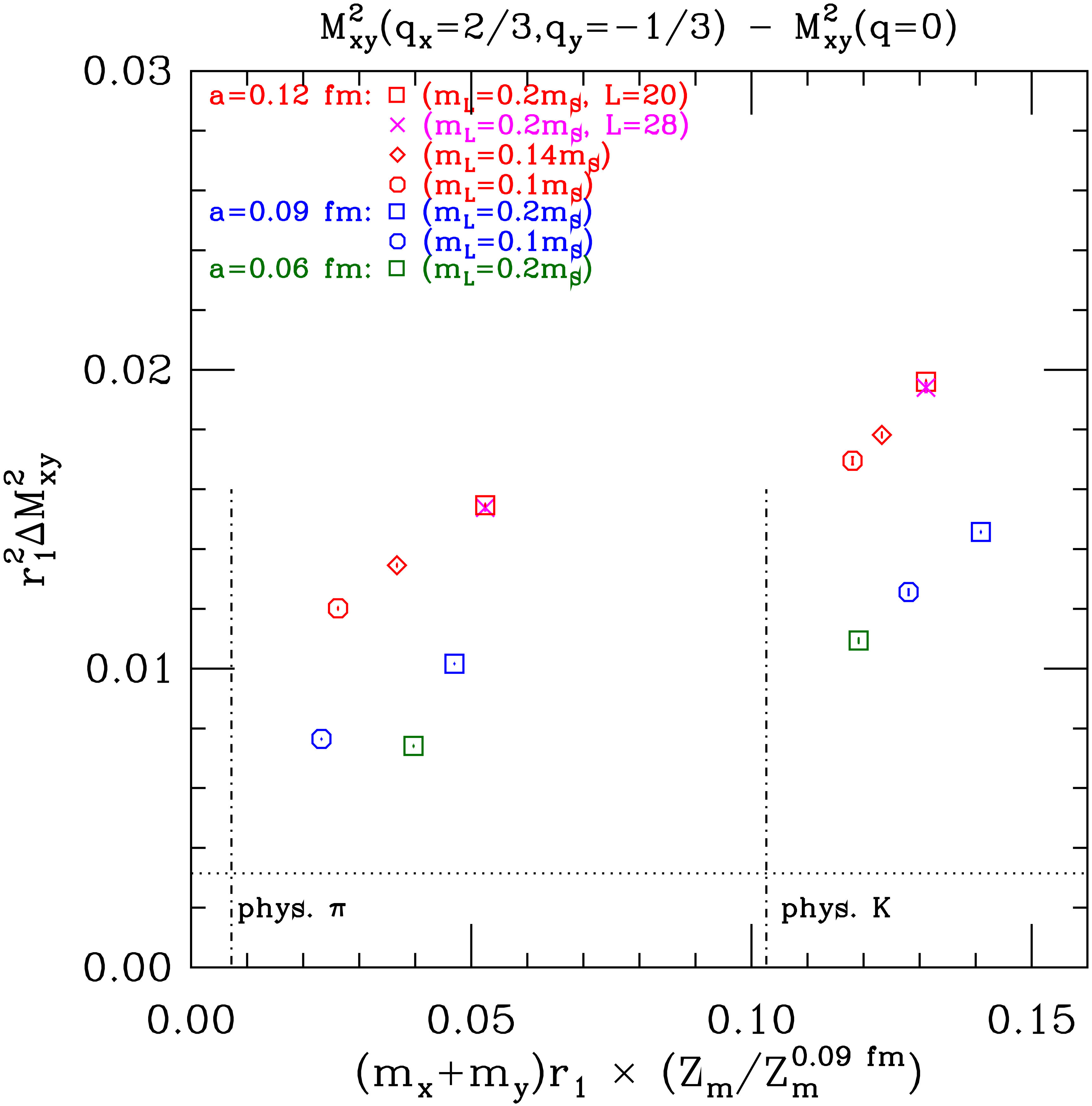

- Points after correction for finite-volume effects.
- Correction is ~7--10% (pions) and ~10--18% (kaons).
  - *Bigger* correction at higher mass because of overall factor of m^2 in 1-loop diagrams, but not at LO (Dashen's theorem).
- Note that $a \simeq 0.12$ fm, $m_l \simeq 0.2 m_s$ points for L=20 (□) and L=28 (×) are consistent.

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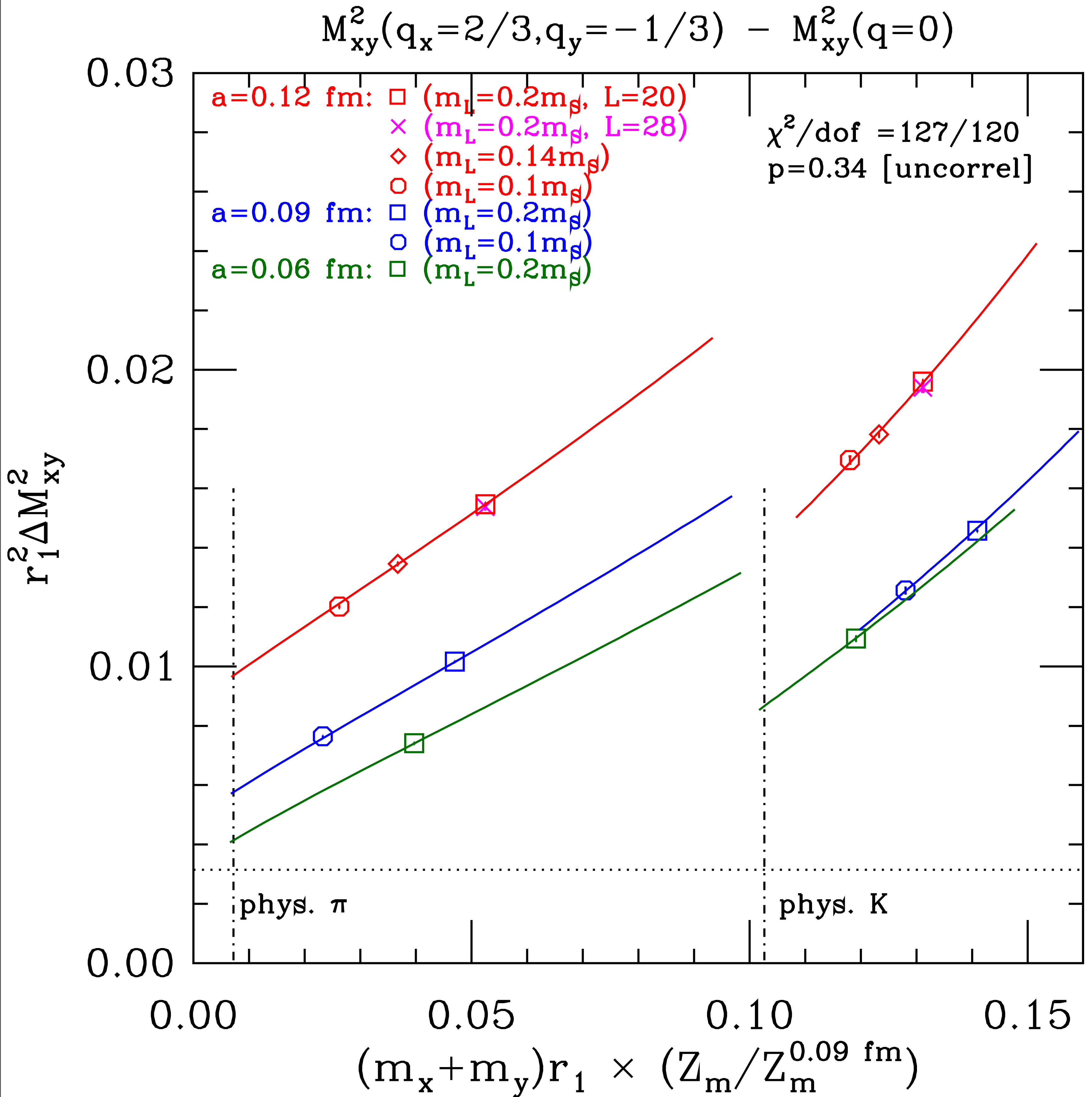
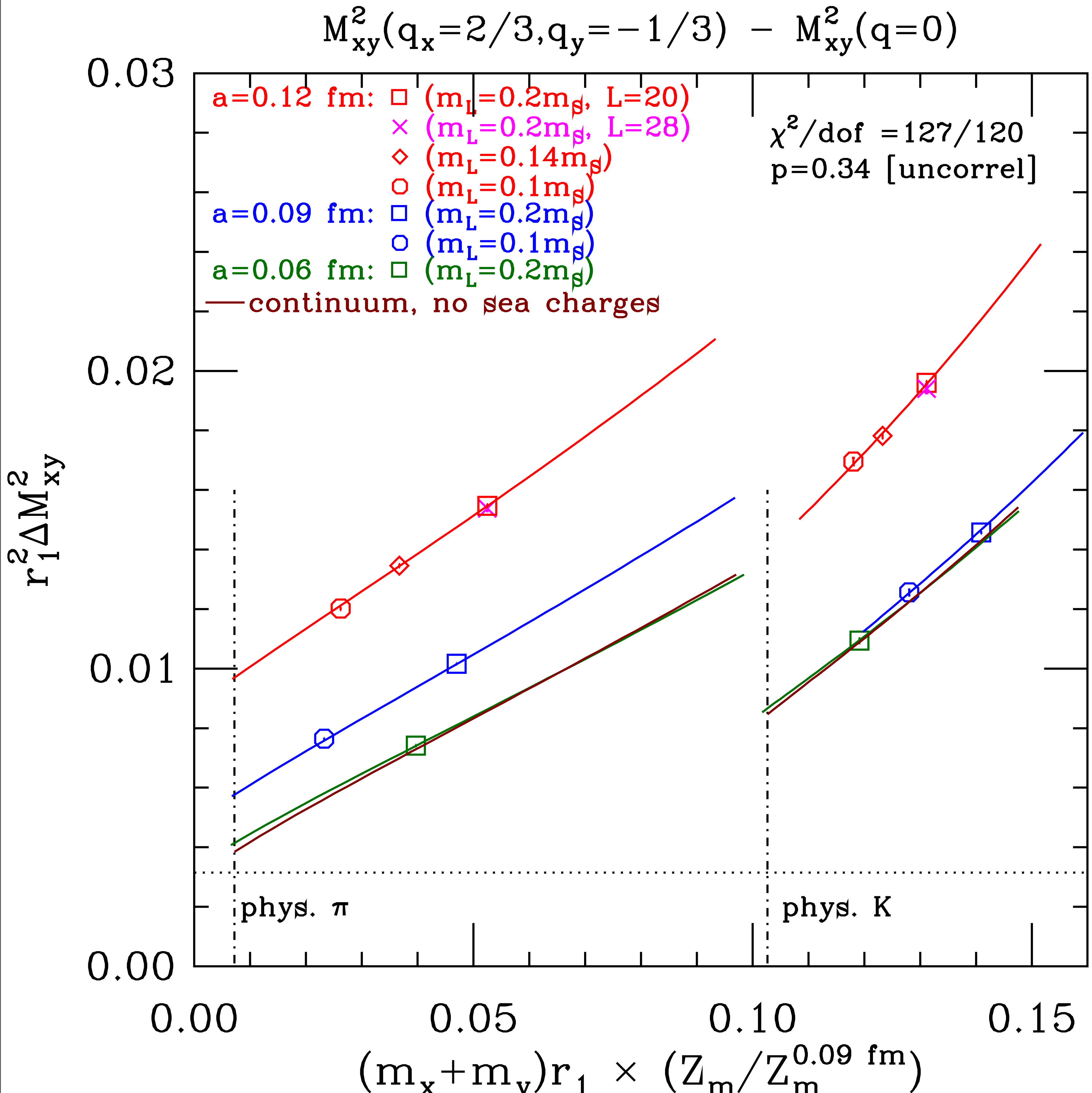


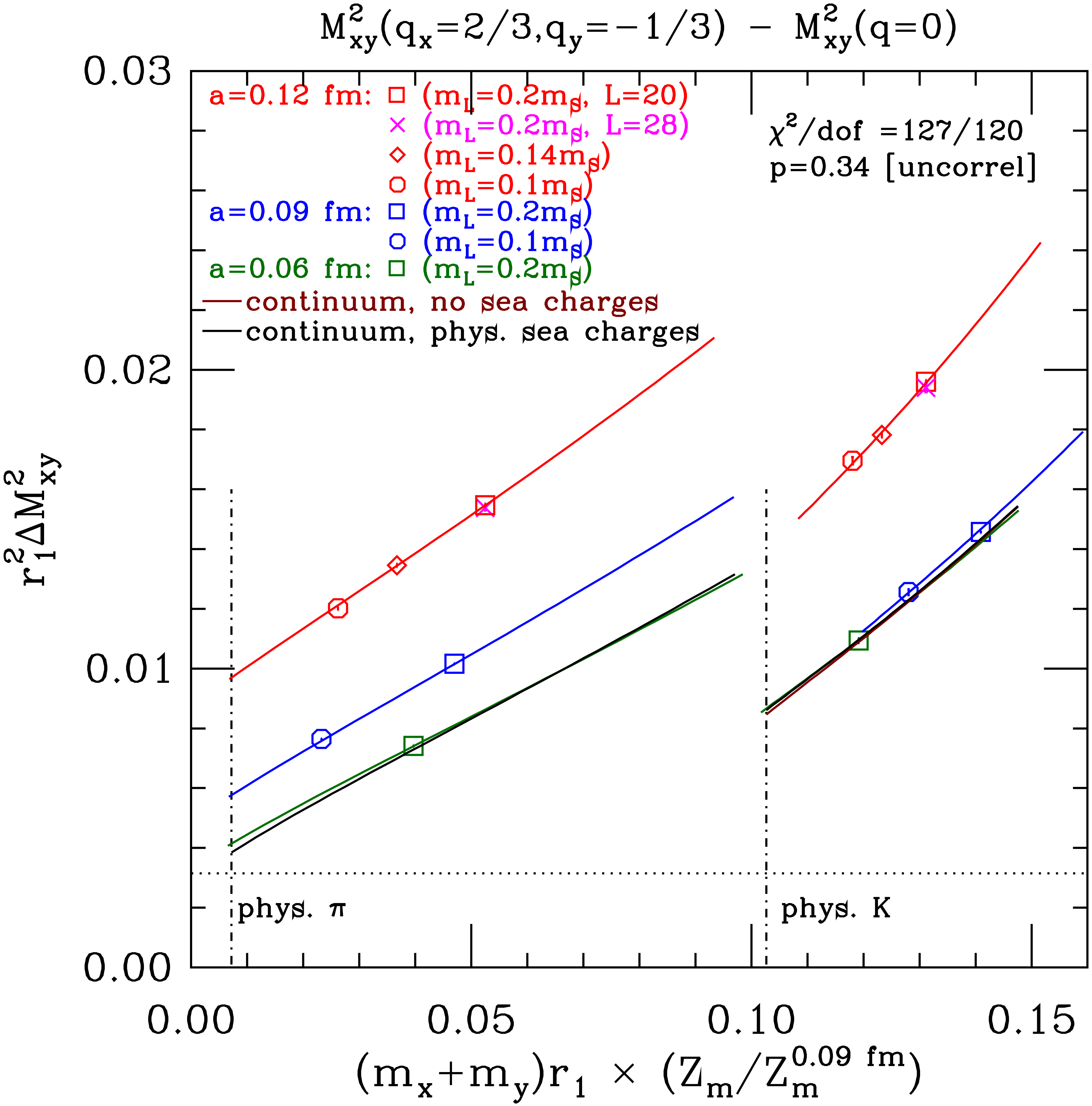
- Chiral fit to infinite-volume (corrected) points.
- Data has very high correlations for different valence masses or charges on the same ensembles: covariance matrix nearly singular.
- For that reason, and because errors are tiny (0.4--0.8%), it is difficult to get decent correlated fits.
- This is a uncorrelated fit; has 149 data points, 29 parameters, χ^2/dof=127/120, p=0.34.
- Fits are generally significantly better than earlier ones without FV corrections.

Chiral Fit and Extrapolation



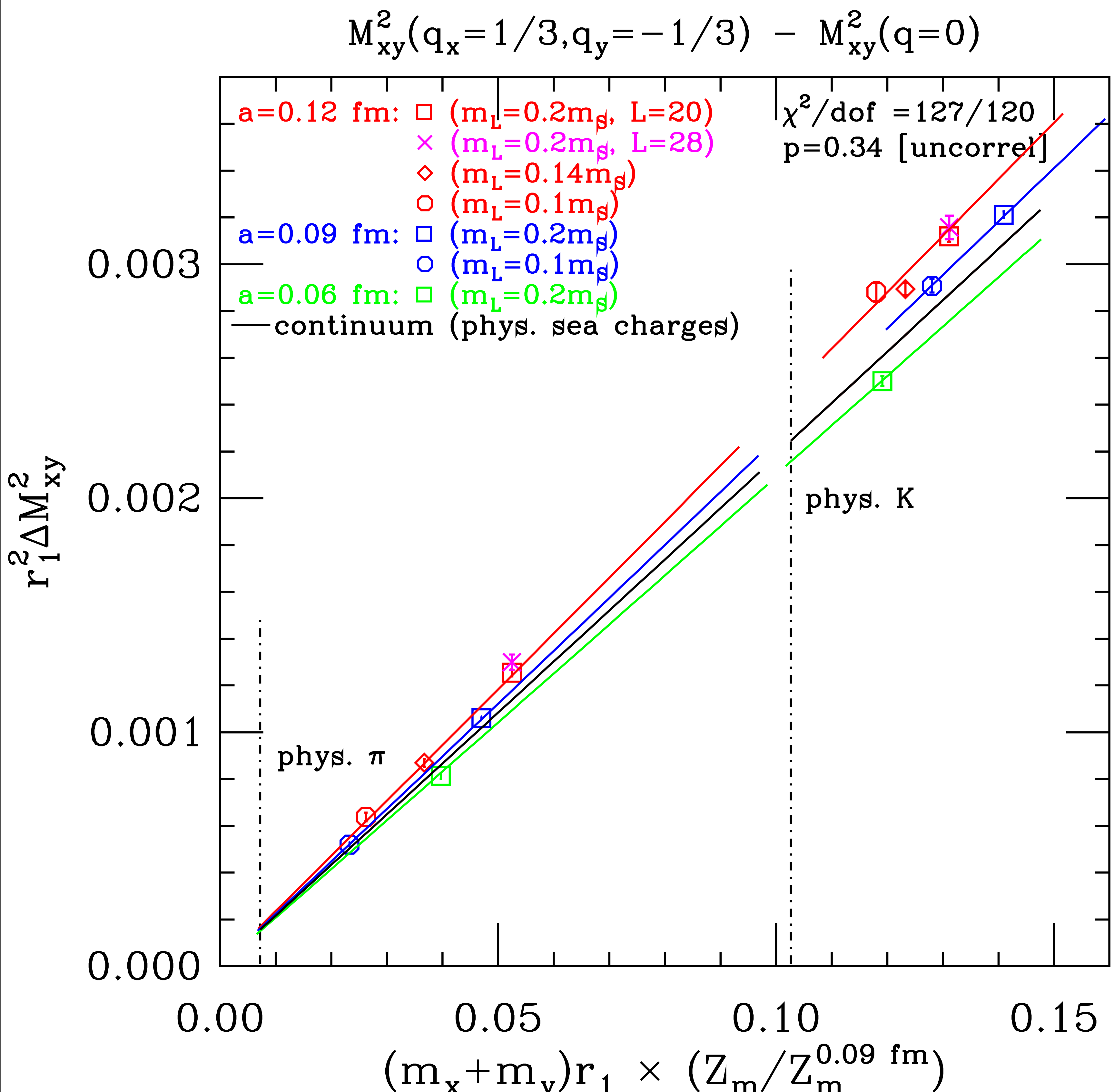
- Extrapolate to continuum, and set valence, sea masses equal.
- Adjust m_s to physical value.
- Keep sea charges = 0.
- Small change between a=0.06 fm and continuum is conspiracy between discretization and m_s effects.

Chiral Fit and Extrapolation



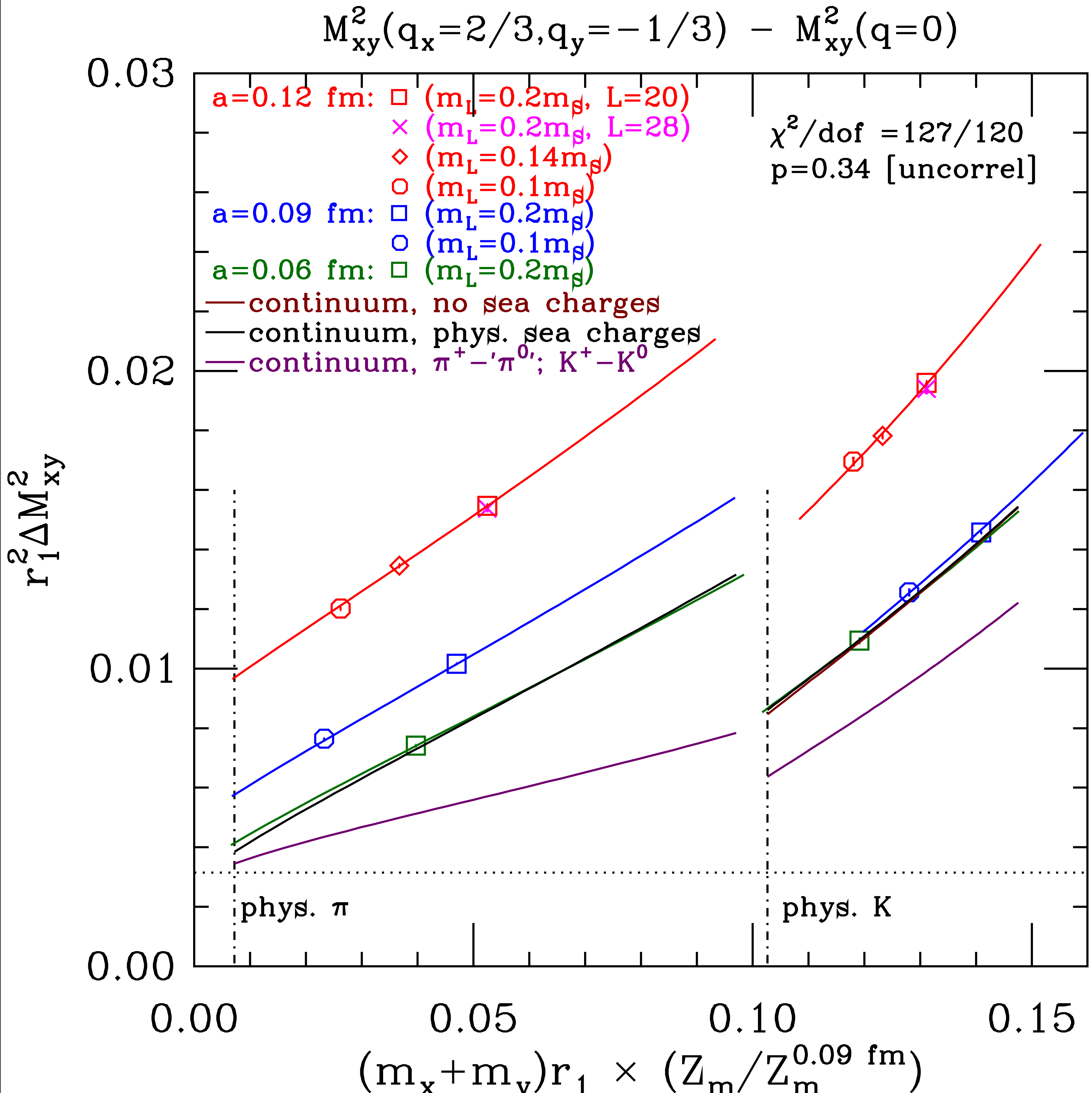
- Set sea quark charges to their physical values, using NLO chiral logs.
- Difference with previous case is very small for kaon; vanishes identically for pion.

Chiral Fit and Extrapolation



- Neutral $d\bar{d}$-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 (π and K line up).
- Nearly linear: chiral logs vanish for neutrals.

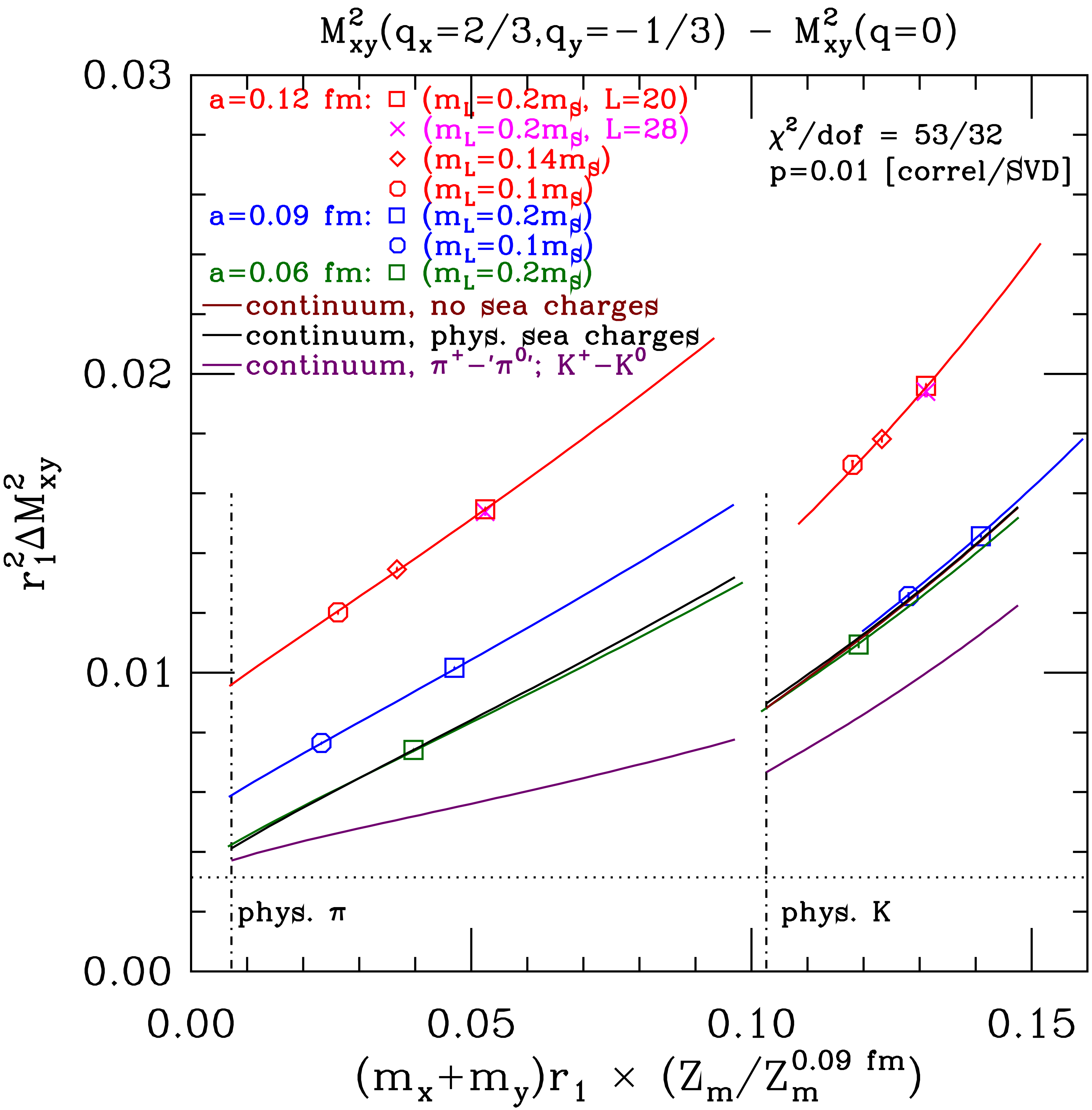
Chiral Fit and Extrapolation



- Now subtract neutral masses from charged masses to give purple lines.
- We are not including disconnected EM graphs for π^0, which is why we call it 'π^0'.
- Horizontal dotted line shows experimental value of π splitting; difference between it and intercept of purple line with vertical, dashed-dotted physical π line is a measure of systematic errors.
- Can now read off ratio of K and π splittings:

$$\epsilon = 0.84(5)$$

Chiral Fit and Extrapolation



- 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, χ^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 ϵ 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 ϵ 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 ϵ by ratio of results for K and π splittings, we may use the experimental π splitting. This gives ϵ =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 π^0.

Current Result

- Get (preliminary!):

$$\epsilon = 0.84(5)_{\rm stat}(18)_{a^2}(10)_{\rm FV}$$

or:

$$\epsilon = 0.84(21)$$

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

$$m_u/m_d = 0.4482(48)_{\rm stat}\left({}^{+\ 21}_{-115}\right)_{a^2}(1)_{\rm FV_{QCD}}(177)_{\rm EM}$$

  - where here "EM" denotes all errors from ϵ, while "FV_{QCD}" refers to finite-volume effects in the pure QCD calculation on the HISQ ensembles.

Future Plans

✦ We have data from additional ensembles at $a \simeq 0.06$ fm and $a \simeq 0.045$ 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:

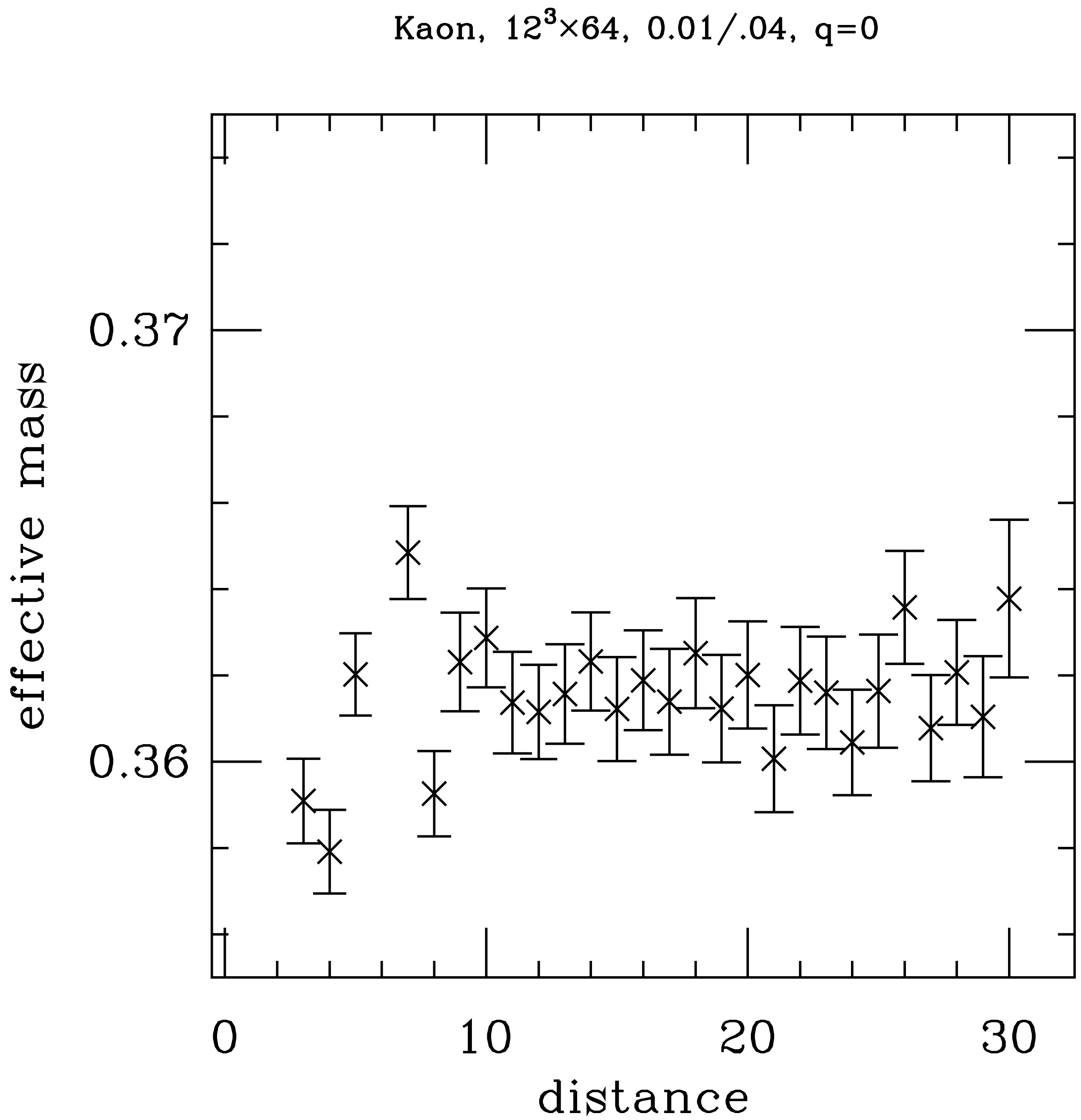
- Smaller discretization effects.
- Nearly absent chiral extrapolation errors, since ensembles with physical masses are included.
- Smaller FV effects, since our HISQ lattices are generally larger than the older asqtad ones. Max size ~5.5 fm.

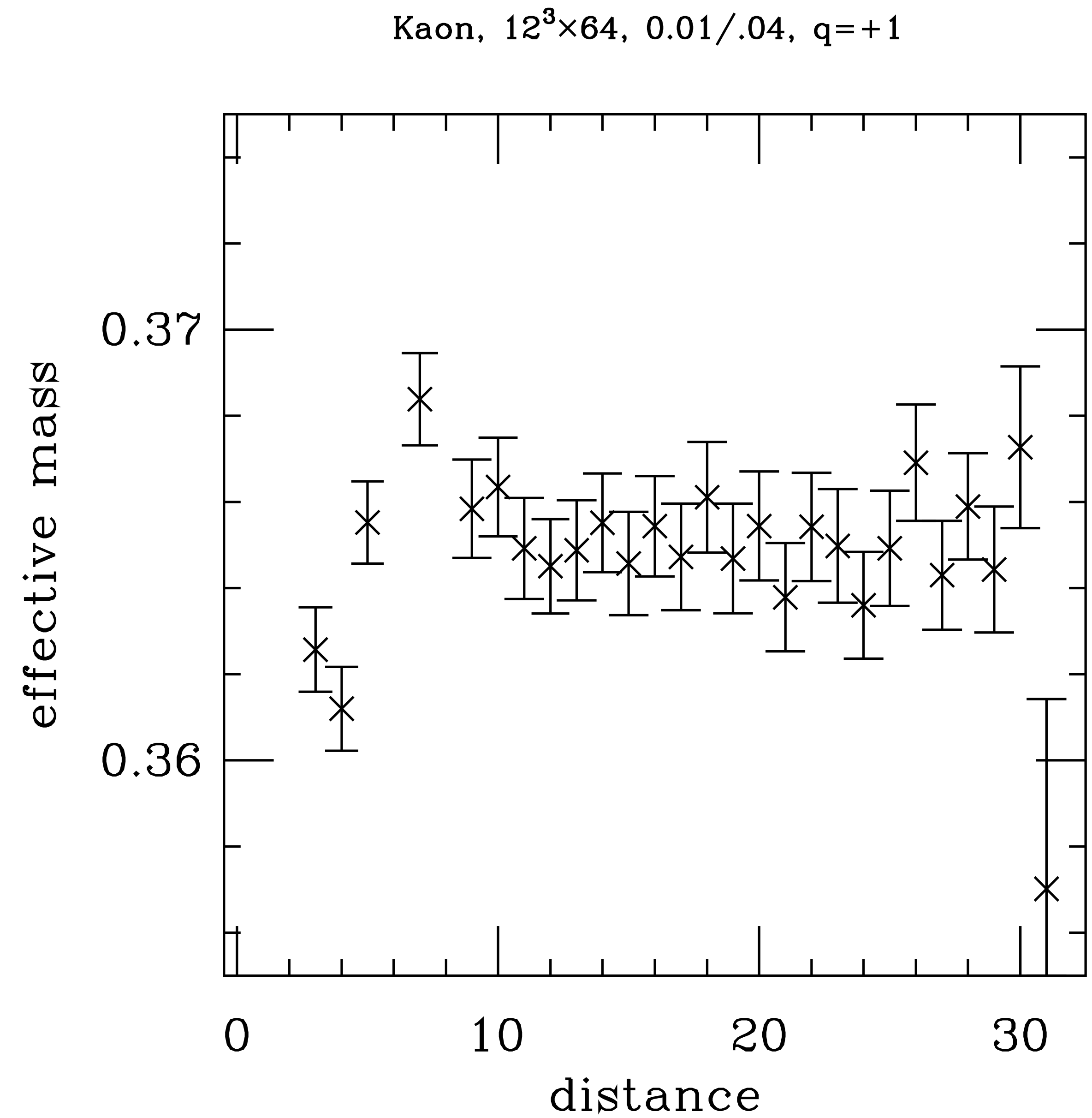
✦ Extension to unquenched case will make possible controlled calculations of many additional quantities.

- Dynamic (unquenched) QED code has been written, and has passed some basic tests.

Back-up Slides

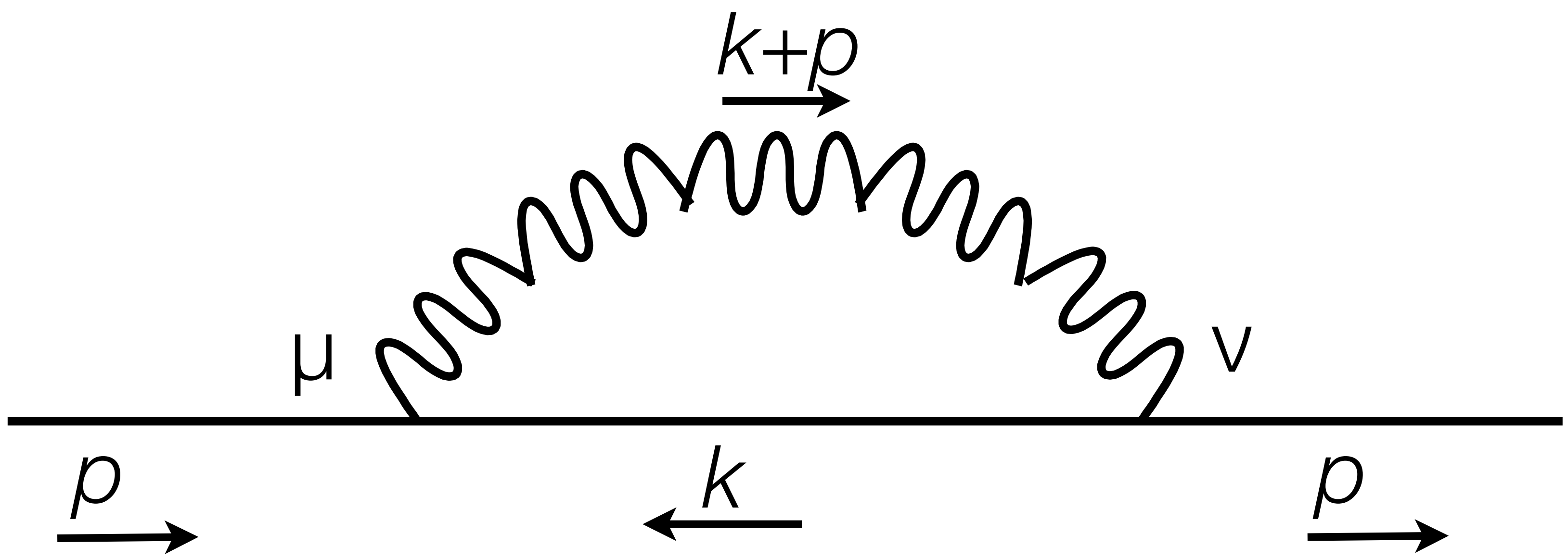
Effective Mass Plots





- 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.

Finite-Volume ChPT: Sunset Graph



✦ In rest frame, $p = (p_0,0,0,0)$, only the 00 component of the photon propagator contributes.

✦ In infinite-volume, get:

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

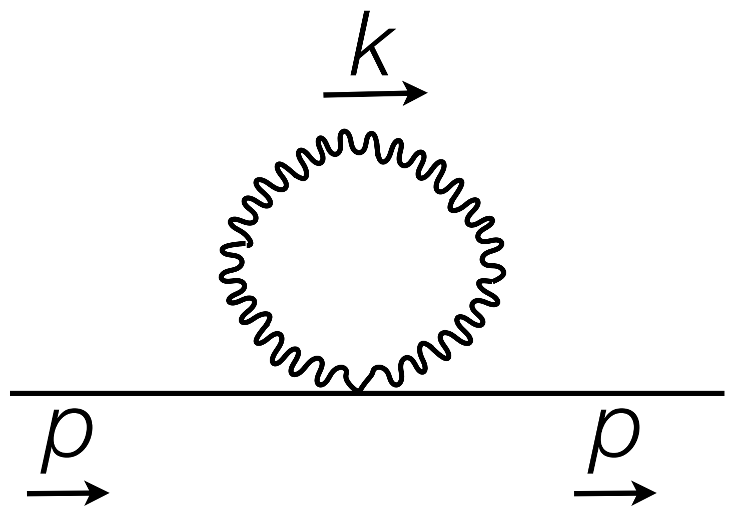
- where m is the meson mass, and numerator comes from momentum factors in the coupling of a (pseudo)scalar particle to a photon.

Finite-Volume ChPT: Sunset Graph

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

- k_0 integral, by itself, is linearly divergent.
- Even when we take difference between finite (spatial) volume version ["FV"] and infinite (spatial) volume version ["∞V"], the k_0 integral makes the difference linearly divergent.
- (Usually, all divergences are the same in FV and ∞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.

Finite-Volume ChPT: Photon Tadpole



- 00 piece of photon propagator gives: $$-\int \frac{d^4k}{(2\pi)^4}\frac{1}{\vec{k}^2}$$
- Combines with sunset to give:

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

- 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.

FV Corrections: Comparison

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