Slow topology change and its effects

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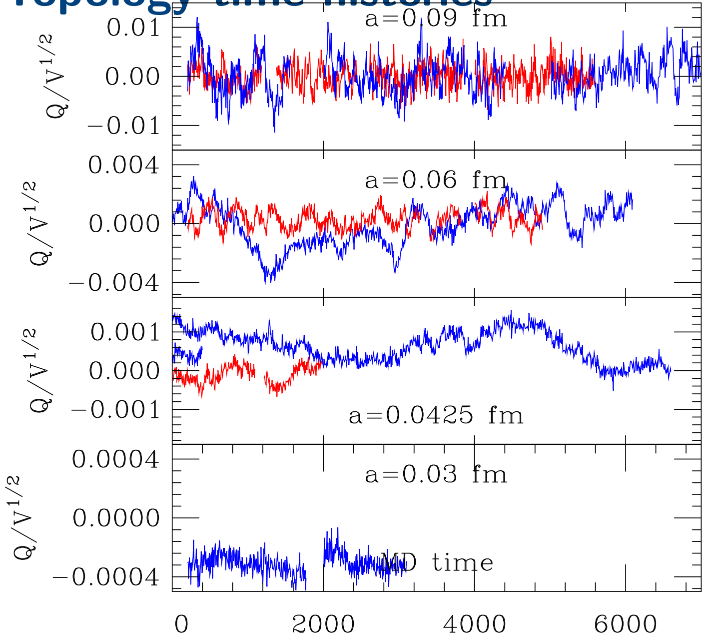
Introduction

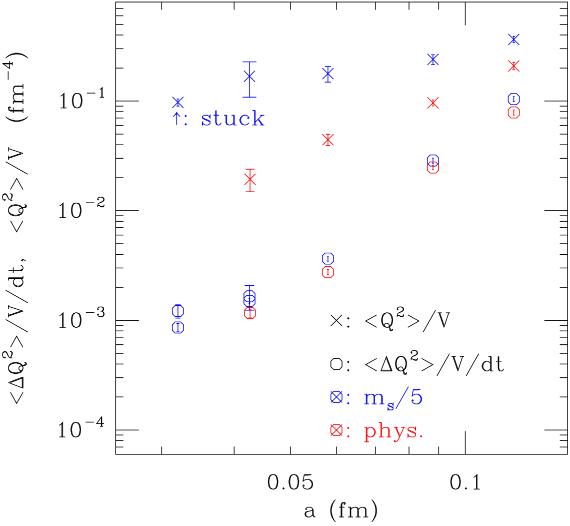
- Evolution of topology gets very slow as $a \longrightarrow 0$
- How slow?
- Does it affect M_{ps} and F_{ps}?
- How should we account for it?
- Work in progress — we haven't really adjusted data yet

Topology time histories



- Q histories
- $m_l =$ physical
- $m_l = m_s/5$
- Notice narrower distributions and shorter autocorrelation time for physical quark mass.

χ_T



- Crosses: $< Q^2/V >$
- Octagons: Tunneling rate $\langle(\Delta Q)^2\rangle$ decreases as $a \to 0$, more or less independent of mass.
- But width of Q distribution smaller for smaller mass, so takes less time to cover the distribution.

Theory basics

- Definition of θ and topological susceptibility χ_t

$$Z(\theta) \;=\; \int \mathcal{D}A\mathcal{D}\bar{\Psi}\mathcal{D}\Psi \;\exp(-S[A,\bar{\Psi},\Psi])\exp(-i\theta Q[A])$$

$$\chi_t \;\equiv\; -\frac{1}{V}\left(\frac{1}{Z}\frac{\partial^2 Z}{\partial\theta^2}\right)\Bigg|_{\theta=0} = \;\frac{1}{V}\langle Q^2\rangle$$

- Fourier transform on θ gets quantities at fixed Q:

$$Z_Q \;=\; \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \;\exp(i\theta Q)Z(\theta)$$

$$G_Q \;=\; \langle \mathcal{O}_1\mathcal{O}_2 \ldots \mathcal{O}_n\rangle_Q = \frac{1}{Z_Q}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta \;\exp(i\theta Q)Z(\theta)G(\theta)\rangle_\theta$$

with $G(\theta) = \langle \mathcal{O}_1\mathcal{O}_2 \ldots \mathcal{O}_n\rangle_\theta$

[Leutwyler and Smilga 1992, Brower *et al.* 2003, Aoki *et al.* 2007, Dromard *et al.* 2015]:

Properties at fixed Q

- For large 4-dim volumes V, we can do θ integrals by saddle point method

$$G_Q = G(\theta_s) + \frac{1}{2\chi_t V}\frac{\partial^2 G}{\partial\theta^2}\Big|_{\theta=\theta_s} + ..., \quad \text{with } \theta_s = i\frac{Q}{\chi_t V}$$

- This gives, for particle mass M and decay constant f:

$$\begin{aligned} M\big|_{Q,V} &= M + \frac{1}{2\chi_t V}M''\left(1 - \frac{Q^2}{\chi_t V}\right) + \mathcal{O}\left(\frac{1}{(\chi_t V)^2}\right) \\ f\big|_{Q,V} &= f + \frac{1}{2\chi_t V}f''\left(1 - \frac{Q^2}{\chi_t V}\right) + \mathcal{O}\left(\frac{1}{(\chi_t V)^2}\right) \end{aligned}$$

where $B'' \equiv \frac{\partial^2 B}{\partial\theta^2}\Big|_{\theta=0}$ for any quantity B.

- $\langle Q^2\rangle = \chi_t V$, $\rightarrow$ correction vanishes when averaged over Q^2.

[Leutwyler and Smilga 1992, Brower *et al.* 2003, Aoki *et al.* 2007, Dromard *et al.* 2015]:

Properties at fixed Q, continued

- M'' and f'' are physical:
    - Can evaluate them on one ensemble to estimate effects on another.
    - Can also calculate them in continuum, infinite volume, ChPT.
- These methods allow us to estimate errors in M and F due to problems in our sampling of the topological-charge distribution, or even make corrections for poor sampling.

ChPT in unitary case

- With an anomalous chiral rotation, can get rid of $i\theta Q$ term in action and put into quark mass matrix.
- Chiral Lagrangian for n_F flavors becomes:

$$\mathcal{L} = \frac{f^2}{8}\mathrm{tr}(\partial_\mu \Sigma \partial_\mu \Sigma^\dagger) - \frac{Bf^2}{4}\mathrm{tr}(e^{-i\theta/n_F}\mathcal{M}\Sigma + e^{i\theta/n_F}\mathcal{M}\Sigma^\dagger)$$

- At tree level, we need to minimize the potential energy term to find $\langle \Sigma \rangle$ (*i.e.*, the vacuum state).
- Then expand potential to second order in fields to find meson masses as a function of θ.
- Axial current and hence decay constants come only from kinetic energy term; will be independent of θ unless $\langle \Sigma \rangle$ has non-trivial θ dependence.

Brower *et al.* 2003; Aoki & Fukaya, 2009

ChPT calculation in unitary case

- With $n_F = 3$, and $m_u = m_d \equiv m \neq m_s$,

$$\langle \Sigma \rangle = \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & e^{i\alpha} & 0 \\ 0 & 0 & e^{-2i\alpha} \end{pmatrix}$$

- Minimize potential energy to find α. (It's enough to do this implicitly, since we only need derivatives at $\theta = 0$.)
- Expand around vacuum state $\langle \Sigma \rangle$ by

$$\Sigma = \sqrt{\langle \Sigma \rangle}\, e^{2i\Phi/f} \sqrt{\langle \Sigma \rangle},$$

with Φ the meson field.

- This way of expanding keeps "extended parity" (parity+ $\theta \to -\theta$) simple: $\Phi \to -\Phi$, $\Sigma \to \Sigma^\dagger$.

Results in unitary case

- Subsumed in partially quenched case, so skip for now
- With $n_F = 3$, and $m_u = m_d \equiv m \neq m_s$,

$$
\begin{aligned}
M''_\pi &= -M_\pi \frac{m_s^2}{2(m+2m_s)^2}, \\
M''_K &= -M_K \frac{m m_s}{2(m+2m_s)^2}, \\
f''_\pi &= 0, \\
f''_K &= -f_K \frac{(m_s-m)^2}{4(m+2m_s)^2}.
\end{aligned}
$$

- For $n_F = 4$, decoupling works (if m_c is sufficiently heavy), so can use the above results.

ChPT in partially quenched case

- Aoki & Fukaya (2009) worked this out using replica method to remove the determinant of the valence quarks.
- However, the calculation is non-perturbative (need to find a non-trivial vacuum), and the replica method is really only justified perturbatively.
- Lagrangian approach of Bernard & Golterman (1993), which introduces ghost (bosonic) quarks to cancel the valence quark determinant, is also only valid perturbatively:
  - Ignores the requirement that bosonic path integral be convergent.
  - $\Rightarrow$ propagators of ghost-ghost mesons have wrong sign at chiral level.
- Sharpe & Shoresh [SS] (2001) and Golterman, Sharpe, & Singleton [GSS] (2005) fixed the non-perturbative problems of Lagrangian approach by taking into account the requirement of convergence for path integral.

ChPT in partially quenched case

- Chiral field of SS and GSS takes the form (up to subtleties on the diagonal):

$$\Sigma = e^{2i\Phi/f}, \qquad \Phi = \begin{pmatrix} \phi & \bar{\chi} \\ \chi & -i\hat{\phi} \end{pmatrix}$$

  - Quark-quark meson field ϕ is as usual: path integral over compact space.
  - Quark-ghost fields χ and $\bar{\chi}$ are fermionic: path-integral convergence not an issue.
  - Ghost-ghost field $\hat{\phi}$ is bosonic & hermitian, and integrated from $-\infty$ to $+\infty$. (Technically, we mean the "body" of $\hat{\phi}$ here.)
- Chiral Lagrangian for n_F sea quarks (and arbitrary number of valence quarks) is then

$$\mathcal{L} = \frac{f^2}{8}\mathrm{str}(\partial_\mu \Sigma \partial_\mu \Sigma^{-1}) - \frac{Bf^2}{4}\mathrm{str}(e^{-i\theta/n_F}\mathcal{M}\Sigma + e^{i\theta/n_F}\mathcal{M}\Sigma^{-1})$$

  - propagator of $\hat{\phi}$ has correct sign, despite supertrace (str), because of extra -i factors.

ChPT calculation in partially quenched case

- Analysis then proceeds much as in unitary case.
- Key differences:
  - Potential energy is complex! Need to find a saddle point (deforming $\hat{\phi}$ contour as needed), not a minimum.
  - Must demand/check that symmetry between valence and ghost quarks is not spontaneously broken.
- Results, for meson made from valence quarks x and y:

$$M''_{xy} = -M_{xy} \frac{m^2 m_s^2}{2(m+2m_s)^2} \frac{1}{m_x m_y},$$

$$f''_{xy} = = -f_{xy} \frac{m^2 m_s^2}{4(m+2m_s)^2} \frac{(m_x - m_y)^2}{m_x^2 m_y^2}.$$

  - Agrees with Aoki & Fukaya, (2009).
  - Singular limit as $m_x \to 0$ or $m_y \to 0$ presumably comes from topological zero modes: not suppressed by low valence-quark mass since valence determinant absent.

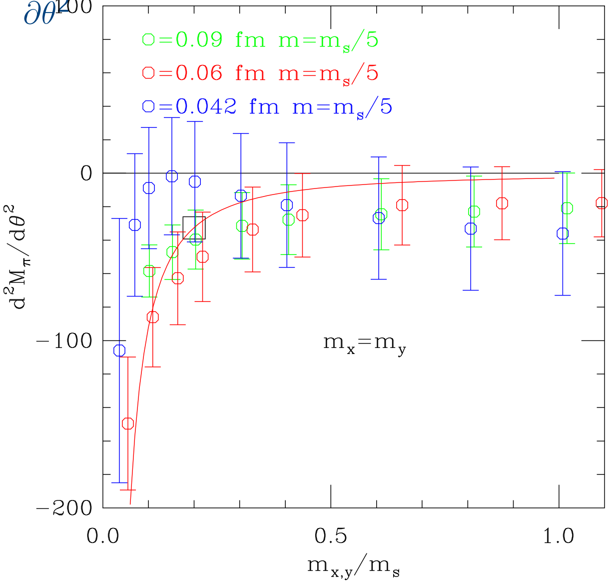
Are we in trouble at small m_l?

- $$M\Big|_{Q,V} \;=\; M + \frac{1}{2\chi_t V} M'' \left(1 - \frac{Q^2}{\chi_t V}\right) + \mathcal{O}\left(\frac{1}{(\chi_t V)^2}\right)$$
- Dependence on quark mass? $\chi_t \propto m_l$, but we increase L as $m_l \to 0$: $V \propto M_\pi^{-4} \propto m_l^{-2}$
- Roughly, prefactor $\frac{1}{2\chi_t V} \propto m_l$
- For M'' and F'', fractional effects ind. of m_l (unitary case)
- Better on the physical quark mass ensembles!
- And also, Q equilibrates faster on physical quark mass ensembles

Test χPT with our data

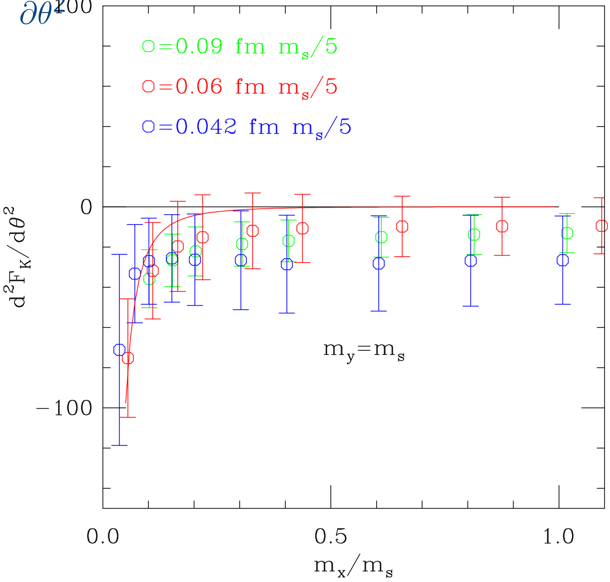
- Reconstruct effective M_π and F_π for each lattice from single elimination jackknife. ($-N$ times deviation of jackknife sample average)
- Error on each point = std. dev. of distribution, so $\chi^2/D = 1$ for fit to constant (*i.e.* average)
- Linear fit: $M_\pi = M_0 + \frac{C}{2} Q^2$.
- Find $\frac{\partial^2 M}{\partial \theta^2}$ from $C = \frac{\partial M_\pi}{\partial Q^2}$.
- Decrease in χ^2/D is fraction of variance attributable to changes in Q^2.
- (This reverse engineering was checked on 0.06 fm $m_s/5$ ensemble by separately analyzing two parts: $Q^2 >$ above/below median.)

$\frac{\partial^2 M}{\partial \theta^2}$



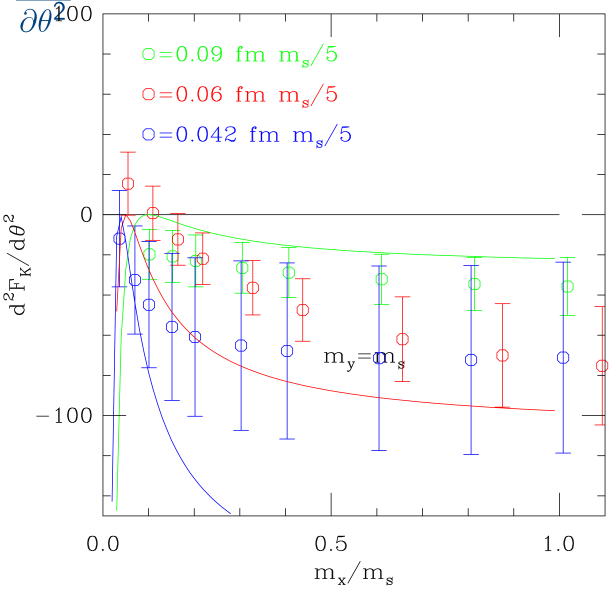
- $\frac{\partial^2 M}{\partial \theta^2}$
- Ensembles with $m_l = m_s/5$
- Along the line $m_A = m_B$
- Line is PQχPT prediction (no free parameters)
- Square is unitary point
- $\sim$ 2 std. dev. at best, but does do the expected thing

$\frac{\partial^2 F}{\partial \theta^2}$



- $\frac{\partial^2 F}{\partial \theta^2}$
- Ensembles with $m_l = m_s/5$
- Along the line $m_B = m_s$
- Line is PQχPT
- (remember it vanishes for degenerate quarks.(

$\frac{\partial^2 F}{\partial \theta^2}$

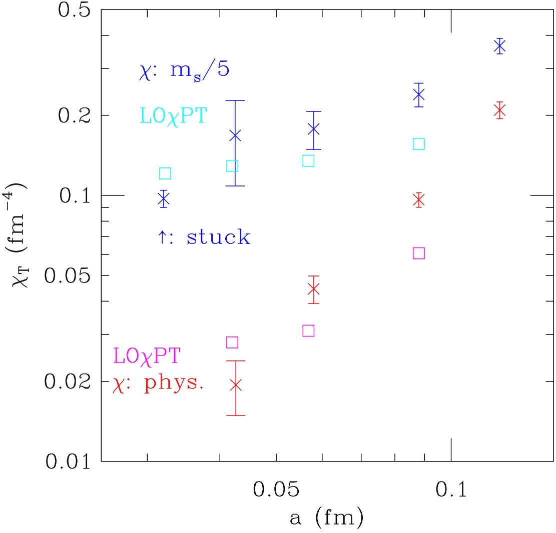


- $\frac{\partial^2 F}{\partial \theta^2}$
- Ensembles with $m_l = m_s/5$
- Along the line m_B = smallest
- Lines are PQχPT
- 3 lines, because ensembles had different smallest m_A

How big are the corrections?

- OK, at $\sim$ two standard deviation level, χPT works — so what?
- If we know the correct $< Q^2 >$, we can adjust our data
- LO staggered χPT: $\chi_T = \frac{f_\pi^2}{4} \overline{M_I^2}$
- where $1/\overline{M_I^2} = 2/M_{\pi,I}^2 + 1/M_{ss,I}^2$ (taste singlet masses)

χ_T



- Crosses are $\frac{Q^2}{V}$ in our simulations
- Squares are lowest order staggered χPT
- For large a ($\approx>$ 0.9 fm) LO χPT doesn't work well.

Example 1: f_K/f_π at $a = 0.042$ fm, m_{phys}

- Physical quark mass ensemble
- $f_{corrected} = f_{sample} - \frac{1}{2\chi_T V} F'' \left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right)$
- L=6.05 fm: $\frac{1}{2\chi_T V} = 0.013$
- χPT: $F'' = -0.055\, F$
- χPT: $\chi_T = 0.028\ \mathrm{fm}^{-4}$, $< Q^2 >_{sample} / V = 0.020$, $\left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right) = 0.29$
- $\frac{\Delta f}{f} = 0.0002$
- *cf* fractional statistical error on $f_K/f_\pi = 0.0010$
- *cf* "conventional" finite size effect (NNLO SχPT), (fractional) 0.0009

Example 2: f_K/f_π at $a = 0.042$ fm, $m_l = m_s/5$

- OK, try an unphysical quark mass ensemble
- Look at lightest valence quark, $m \approx m_{phys}$
- Worst case – a PQ divergence here
- $f_{corrected} = f_{sample} - \frac{1}{2\chi_T V} F'' \left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right)$
- L=2.88 fm: $\frac{1}{2\chi_T V} = 0.07$
- χPT: $F'' = -0.10\, F$
- χPT: $\chi_T = 0.129 \text{ fm}^{-4}$, $< Q^2 >_{sample} / V = 1.30$, $\left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right) = -0.30$
- $\frac{\Delta f}{f} = -0.002$
- *cf* fractional statistical error on $f_K/f_\pi = 0.003$

Comment on strategy

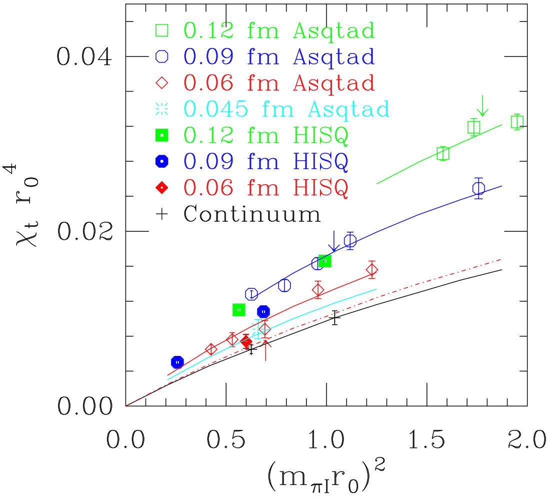
- This is really the same general strategy that we use for "conventional" finite size effects:
- Use χPT to estimate the effects.
- Check χPT against a simulation someplace where it is possible
- Adjust results using χPT.
- Systematic error budget includes estimate of residual effects: higher order χPT and/or uncertainties in χPT parameters.
- To be fair, we have not yet included these corrections in talks at this conference — still a work in progress.
- And χPT hasn't been done for other things, *e.g.* heavy-light

EXTRA SLIDES

Example 3: f_K/f_π at $a = 0.032$ fm, $m_l = m_s/5$

- Another unphysical quark mass, Q almost stuck in this one.
- Did not run light PQ correlators on this one, so "f_π" is at $m_s/5$
- $f_{corrected} = f_{sample} - \frac{1}{2\chi_T V} F'' \left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right)$
- L=3.09 fm: $\frac{1}{2\chi_T V} = 0.046$
- χPT: $F'' = -0.033\, F$
- χPT: $\chi_T = 0.121\ \mathrm{fm}^{-4}$, $< Q^2 >_{sample} / V = 0.097$, $\left(1 - \frac{<Q^2>_{sample}}{\chi_T V}\right) = 0.20$
- $\frac{\Delta f}{f} = 0.0003$
- *cf* fractional statistical error on $f_K/f_\pi = 0.0016$

Topological susceptibility



- arXiv:1003.5695, 1004.0342
- Really does improve the gauge configurations!!
- (Other tests involve valence quarks)

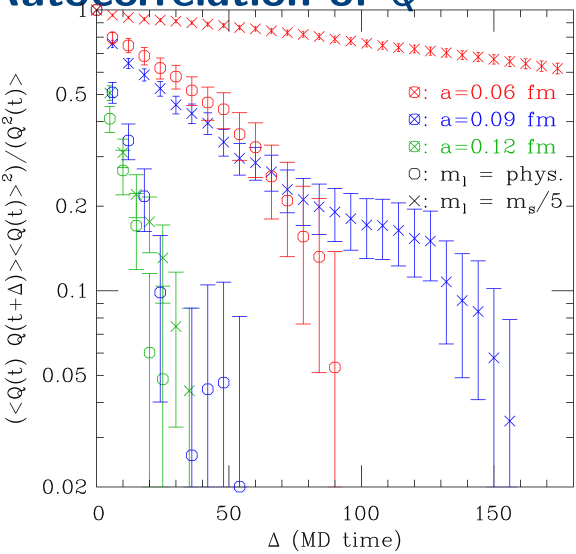
Diagonal fields in partially quenched ChPT

- Fields on the diagonal of Φ correspond to non-anomalous generators, *i.e.*, generators whose supertrace vanishes:

$$
\begin{aligned}
T_1 &= \mathrm{diag}(1,-1,0,0,0,0,0) \\
T_2 &= \mathrm{diag}(1,1,-2,0,0,0,0) \\
T_3 &= \mathrm{diag}(0,0,0,1,-1,0,0) \\
T_4 &= \mathrm{diag}(1,1,1,-3/2,-3/2,0,0) \\
T_5 &= \mathrm{diag}(0,0,0,0,0,1,-1) \\
T_6 &= \mathrm{diag}(1,1,1,1,1,5/2,5/2)
\end{aligned}
$$

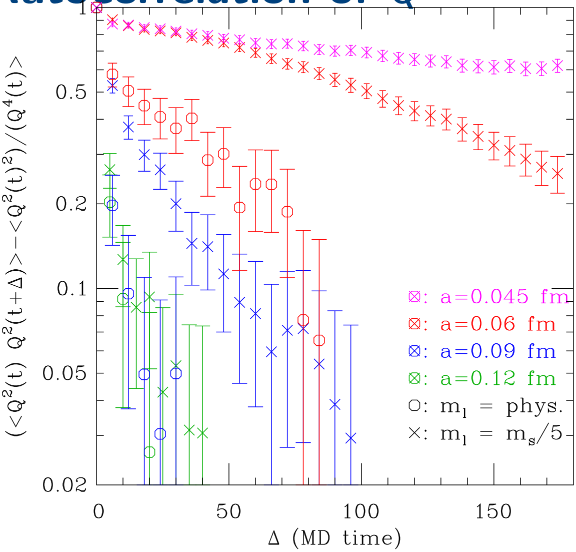
  - Notation: first 3 entries correspond to sea quarks, the next 2 to valence quarks, and the last 2 to ghosts.
- T_1, T_2, T_3, T_4 are quark-like ("normal") since have $\mathrm{str}\, T_i^2 > 0 \Rightarrow$ corresponding fields are real.
- T_5, T_6 are ghost-like since have $\mathrm{str}\, T_i^2 < 0 \Rightarrow$ corresponding fields are $-i \times$ real.

Autocorrelation of Q



- Two hyp smearings, then integrate $F\widetilde{F}$.
- τ increases as a decreases (compare ×,×,×
- τ decreases as m decreases (compare ×,○ or ×,○ .
- Errors in this section VERY approximate

Autocorrelation of Q^2



- Don't usually care about $Q \leftrightarrow -Q$ (CP), so don't care about sign of Q, so look at autocorrelation of Q^2.
- Shorter autocorrelation times, with same general pattern