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**Twisting vs. Staggering: is  
twisted-mass lattice QCD a viable  
alternative to improved staggered  
fermions?**

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**Stephen R. Sharpe and Jackson Wu**

University of Washington

# Outline

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- Introduction: status of lattice fermion actions
- What is twisted-mass lattice QCD (tmLQCD) and why is it interesting?
- Effective chiral Lagrangian for tmLQCD including discretization errors
- Results for “generic small mass” regime:  $m_q \sim a\Lambda_{\text{QCD}}^2$
- Results for “Aoki” regime:  $m_q \sim a^2\Lambda_{\text{QCD}}^3$
- Summary and outlook

# Introduction

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- Lattice QCD is entering an exciting era
  - Terascale computers (e.g. UKQCD's QCDOC)
  - Unquenched simulations with  $m_\pi \rightarrow 250$  MeV and below
  - Potential for few percent control over all systematics
- Choices for light fermion action:
  - Improved staggered fermions
    - Fastest, but not unitary, and possibly not local, at  $O(a^2)$
  - Chirally symmetric fermions
    - The ultimate choice, but slowest
  - Improved Wilson fermions
    - Straightforward, but slow
  - Twisted-mass
    - Maybe as fast as staggered, but potential not yet clear
- **Are twisted-mass fermions a viable alternative to staggered fermions?**

# tmLQCD

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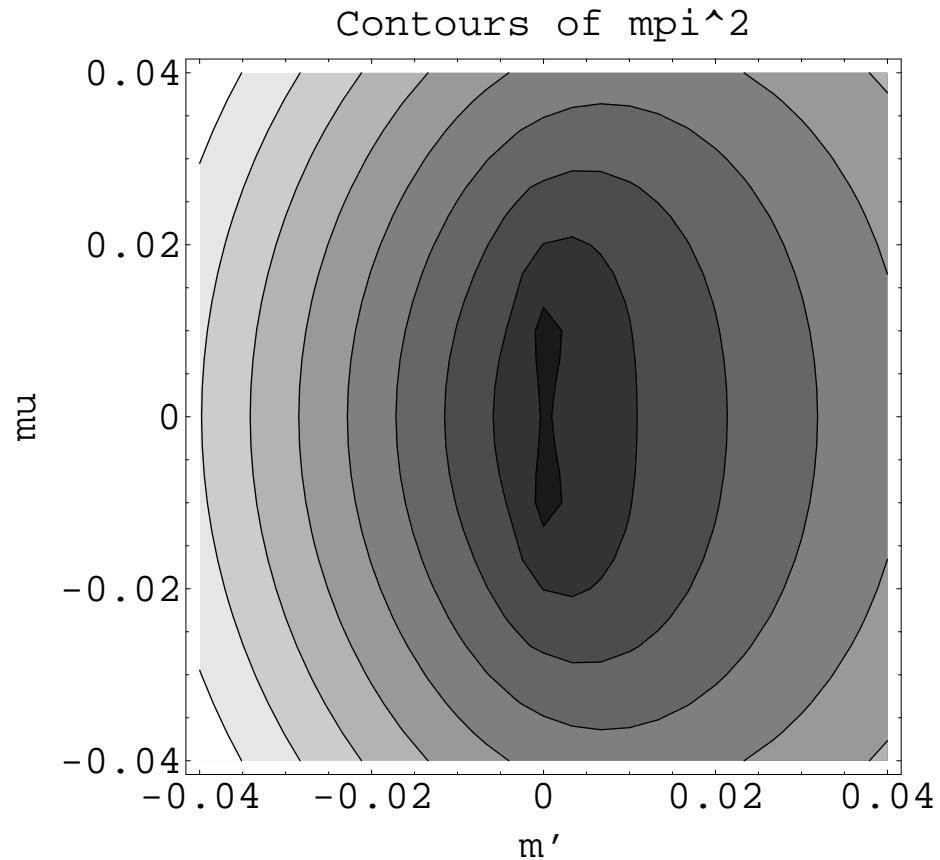
Variant of unimproved Wilson fermions with twisted mass  
[Frezzotti, Grassi, Sint & Weisz, 2000]

- Advantages
  - + WYSIWYG: no roots of determinant
  - + speed comparable to staggered
  - + at “maximal twist”
    - errors  $\sim a^2$  automatically [Frezzotti & Rossi, 2003]
    - operator mixing as in continuum [Frezzotti & Rossi, 2004]
- Disadvantages
  - flavor is broken for  $a \neq 0$ :  $SU(2) \rightarrow U(1)$

**Detailed numerical studies underway** [DESY-Zeuthen]

**We use analytical methods to study its properties**

# What happens to Istvan's circles?



Contour plot of charged  $m_{\pi}^2$  from  $tm_{\chi}PT$  with parameters roughly tuned to match those of hep-lat/0410031, Farchioni *et al.*

# What is tmLQCD?

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Begin in the continuum.

- Action in “twisted basis” for two degenerate flavors ( $\tau_3^2 = 1$ ):

$$\mathcal{L}_{tm} = \bar{\psi}(\not{D} + m_q e^{i\gamma_5 \tau_3 \omega})\psi = \bar{\psi}(\not{D} + m + i\gamma_5 \tau_3 \mu)\psi$$

$$\cos \omega = m/m_q, \quad \sin \omega = \mu/m_q, \quad m_q = \sqrt{m^2 + \mu^2}$$

- Maximal twist is  $m = 0, \omega = \pi/2$ .
- Flavor-breaking is fake: non-singlet axial transformation

$$\hat{\psi} = \exp(i\gamma_5 \tau_3 \omega/2)\psi, \quad \hat{\bar{\psi}} = \bar{\psi} \exp(i\gamma_5 \tau_3 \omega/2)$$

brings  $\mathcal{L}$  into usual form (“physical basis”):

$$\mathcal{L}_{tm} = \hat{\bar{\psi}}(\not{D} + m_q)\hat{\psi}$$

# Kinematics of continuum tmQCD

Currents and densities:

$$A_\mu^j = \bar{\psi} \gamma_\mu \gamma_5 \tau_j \psi, \quad V_\mu^j = \bar{\psi} \gamma_\mu \tau_j \psi, \quad P^j = \bar{\psi} \gamma_5 (\tau_j / 2) \psi, \quad S^0 = \bar{\psi} \psi$$

Relation between operators in twisted and physical bases  
( $a = 1, 2$ ):

$$\begin{aligned} \hat{A}_\mu^a &= \cos \omega A_\mu^a + \epsilon^{3ab} \sin \omega V_\mu^b, & \hat{A}_\mu^3 &= A_\mu^3, \\ \hat{V}_\mu^a &= \cos \omega V_\mu^a + \epsilon^{3ab} \sin \omega A_\mu^b, & \hat{V}_\mu^3 &= V_\mu^3, \\ \hat{P}^3 &= \cos \omega P^3 + i \sin \omega S^0 / 2, & \hat{P}^a &= P^a, \\ \hat{S}^0 &= \cos \omega S^0 + 2i \sin \omega P^3 \end{aligned}$$

Note:  $A_\mu^3$  and  $P^a$  create physical pions for all  $\omega$

# What is tmLQCD?

Lattice action [Frezzotti, Grassi, Sint & Weisz] :

$$S_F^L = a^4 \sum_x \bar{\psi}_l(x) \left[ \frac{1}{2} \sum_{\mu} \gamma_{\mu} (\nabla_{\mu}^* + \nabla_{\mu}) + m_0 + i\gamma_5 \tau_3 \mu_0 - \frac{r}{2} \sum_{\mu} \nabla_{\mu}^* \nabla_{\mu} \right] \psi_l(x)$$

- cannot rotate away twist in mass
  - ⇒ parity and flavor broken, though breaking vanishes in naive continuum limit
- Wilson term  $\nabla_{\mu}^* \nabla_{\mu}$  mixes with identity
  - ⇒ usual additive renormalization of  $m_0$ :  $m = Z_m(m_0 - m_c)/a$
- $\mu_0$  is multiplicatively renormalized, like  $m_q$  in continuum:
  - $\mu = Z_{\mu} \mu_0 / a$
- renormalized twist angle and quark mass:
  - $\tan \omega = \mu / m + O(a)$ ,  $m_q = \sqrt{m^2 + \mu^2} + O(a)$



# Computational advantage of tmLQCD

Rewrite action:

$$\begin{aligned} S_F^L &= a^4 \sum_x \bar{\psi}_l(x) \left[ D_W + m_0 + i\gamma_5 \tau_3 \mu_0 \right] \psi_l(x) \\ &= a^4 \sum_x \bar{\psi}_l(x) \gamma_5 \left[ H_W + i\tau_3 \mu_0 \right] \psi_l(x) \end{aligned}$$

with  $H_W$  the Hermitian Wilson-Dirac operator:

$$H_W = \gamma_5 (D_W + m_0) = H_W^\dagger$$

- computational problem: zero eigenvalues of  $H_W$   
⇒ fermion determinant vanishes, slows algorithms
- solved by twisting:  $\mu_0$  provides IR cut-off

$$\det(H_W + i\tau_3 \mu_0) = \prod_{\lambda} (\lambda + i\mu_0)(\lambda - i\mu_0) = \prod_{\lambda} (\lambda^2 + \mu_0^2)$$

- Simulations comparable in speed to staggered fermions  
[Kennedy, Lattice 04]

# Automatic $O(a)$ improvement

Key property of tmLQCD at maximal twist [Frezzotti & Rossi] :

$$Q_{lat} = Q_{cont} \left[ 1 + ca^2 \Lambda_{QCD}^2 + c' a^2 m_q^2 + O(a^4) \right]$$

Why does this work? We will study for  $a \sim m_q$  so

$$a\Lambda_{QCD} \gg am_q \sim a^2$$

- At maximal twist, have  $m_0 = m_c$ , so

$$\begin{aligned} m_0 - \frac{r}{2} \sum_{\mu} \nabla_{\mu}^* \nabla_{\mu} + i\mu\gamma_5\tau_3 &= i\mu\gamma_5\tau_3 + ac'(D_{\mu}^2)|_{cont} + O(a^2) \\ &\longrightarrow \mu - ac'i\gamma_5\tau_3(D_{\mu}^2)|_{cont} + O(a^2) \end{aligned}$$

when rotate to physical basis

$\Rightarrow O(a)$  corrections necessarily violate parity and flavor

$\Rightarrow$  physical (parity-flavor conserving) quantities corrected only at  $O(a^2)$

# Range of validity of automatic improvement

- Possibilities are: ( $a^{-1} = 2 \text{ GeV}$ ,  $\Lambda_{QCD} = 300 \text{ MeV}$ )
  - (A)  $m_q \gg a\Lambda_{QCD}^2 \sim 45 \text{ MeV}$
  - (B)  $m_q \sim a\Lambda_{QCD}^2 \gg a^2\Lambda_{QCD}^3 \sim 7 \text{ MeV}$
  - (C)  $m_q \geq ca^2\Lambda_{QCD}^3 \sim 7 \text{ MeV}$ , with  $c = O(1)$
- Since  $(m_u + m_d)/2 \approx 3 \text{ MeV}$ , want (B) or, better, (C)
- [Frezzotti & Rossi] argue that (A) is needed:
  - Vacuum should be determined by  $O(m_q)$  and not  $O(a)$  effects
- We claim that can relax to (B) with appropriate definition of  $\omega$
- We agree with [Aoki & Bär] that (C) can also hold, although with  $c \neq 0$  in general.

# Our method: $tm\chi PT$

- We study long-distance physics (vacuum & pion properties) using the chiral Lagrangian extended to include discretization errors
  - understand, analytically, competition between  $O(m_q)$  and  $O(a)$  effects
  - interpret and guide simulations (which are in new territory)
- consider 2 light degenerate flavors
  - results valid for 2+1 flavors if  $p^2 \sim m_\pi^2 \ll m_K^2$
- use two step method of [SRS + Singleton, 1998]
  - (1) construct continuum  $\mathcal{L}_{\text{eff}}$  describing lattice theory [Symanzik]
$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{QCD} + a\mathcal{L}_1 + a^2\mathcal{L}_2 + \dots$$
  - (2) construct chiral effective theory for  $\mathcal{L}_{\text{eff}}$
- power counting: work to NLO using  $p^2 \sim m_q \sim a$

# Step 1: effective continuum Lagrangian

Need most general Lagrangian consistent with lattice symmetries, which include

- Parity + discrete flavor ( $\psi_l \rightarrow i\tau_1\psi_l$ )
- Parity +  $\mu_0 \rightarrow -\mu_0$

Result is simple [Münster & Schmidt, SRS & Wu] :

$$\mathcal{L}_0 = \mathcal{L}_{\text{glue}} + \bar{\psi}(\not{D} + m + i\gamma_5\tau_3\mu)\psi$$

$$\mathcal{L}_1 = b_1[g^2(a)]\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi$$

- same as for Wilson fermions aside from twisted mass in  $\mathcal{L}_0$
- other potential operators in  $\mathcal{L}_1$  vanish by LO equations of motion, or are NNLO in our power counting, e.g.  $\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\gamma_5\tau_3\psi$  requires factor of  $a\mu$
- $\mathcal{L}_2$  is same as for Wilson theory [Bär, Rupak, Shoresh] , but can ignore as introduces no additional symmetry breaking

# Step 2: map onto chiral Lagrangian

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\text{glue}} + \bar{\psi}(\not{D} + m + i\gamma_5\tau_3\mu)\psi + ab_1\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi$$

- For  $m = \mu = a = 0$  have  $SU(2)_L \times SU(2)_R$  chiral symmetry:

$$\psi_{L,R} \longrightarrow U_{L,R}\psi_{L,R}, \quad U_{L,R} \in SU(2)_{L,R}$$

- Symmetry broken by mass and  $a$  terms in same way

- $\bar{\psi}(m + i\gamma_5\tau_3\mu)\psi = \bar{\psi}_L\mathcal{M}\psi_R + \bar{\psi}_R\mathcal{M}^\dagger\psi_L$  with

$$\mathcal{M} = m + i\tau_3\mu = m_q \exp(i\omega\tau_3)$$

- $a\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi \propto \bar{\psi}_L\hat{A}\sigma_{\mu\nu}F_{\mu\nu}\psi_R + \bar{\psi}_R\hat{A}^\dagger\sigma_{\mu\nu}F_{\mu\nu}\psi_L$

- $\mathcal{L}_{\text{eff}}$  invariant if treat  $\mathcal{M}$ ,  $\hat{A}$  as spurions:

$$\mathcal{M} \rightarrow U_L\mathcal{M}U_R^\dagger \text{ and } \hat{A} \rightarrow U_L\hat{A}U_R^\dagger$$

$\Rightarrow$  standard  $\chi$ PT analysis can be used for  $\mathcal{M}$  and  $\hat{A}$

[SRS & Singleton; Bär, Rupak & Shoresh]

# Resulting chiral Lagrangian

$$\begin{aligned}
 \mathcal{L}_\chi = & \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4} \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) - \frac{f^2}{4} \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\
 & - L_1 \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger)^2 - L_2 \text{Tr}(D_\mu \Sigma D_\nu \Sigma^\dagger) \text{Tr}(D_\mu \Sigma D_\nu \Sigma^\dagger) \\
 & + L_{45} \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) - L_{68} [\text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi)]^2 \\
 & + W_{45} \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) - W_{68} \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\
 & - W'_{68} [\text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A})]^2 + W_{10} \text{Tr}(D_\mu \hat{A}^\dagger D_\mu \Sigma + D_\mu \Sigma^\dagger D_\mu \hat{A})
 \end{aligned}$$

where

$$\begin{aligned}
 \Sigma & \sim \langle \psi_L \bar{\psi}_R \rangle \longrightarrow U_L \Sigma U_R^\dagger, \quad D_\mu \Sigma = \partial_\mu \Sigma - i\ell_\mu \Sigma + i\Sigma r_\mu, \\
 \chi & = 2B_0(s + ip) \rightarrow 2B_0 \mathcal{M}, \quad \hat{A} \rightarrow \hat{a} = 2W_0 a
 \end{aligned}$$

and constants are not determined by symmetries

- $f$ ,  $B_0$  and  $L_i$  are from continuum  $\chi$ PT
- $W_i$ ,  $W'_i$  are introduced by discretization errors

# tm $\chi$ PT at leading order

Lagrangian takes continuum form if use variable  $\chi' = \chi + \hat{A}$ :

$$\begin{aligned}\mathcal{L}_{\chi, LO} &= \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4} \text{Tr}(\chi^\dagger \Sigma + \Sigma^\dagger \chi) - \frac{f^2}{4} \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\ &= \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4} \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi')\end{aligned}$$

- corresponds to  $O(a)$  shift in  $m$  and  $m_c$ :

$$m \rightarrow m' = m + aW_0/B_0, \quad m_q \rightarrow \sqrt{m'^2 + \mu^2}, \quad \tan \omega_0 \equiv \mu/m', \quad \chi' = 2B_0 m_q e^{i\omega_0 \tau_3}$$

- condensate aligns with  $\chi'$ :

$$\Sigma = \exp(i\omega_0 \tau_3 / 2) \Sigma_{ph} \exp(i\omega_0 \tau_3 / 2), \quad \Sigma_{ph} = \exp(i\vec{\pi} \cdot \vec{\tau} / f)$$

$\Rightarrow$  LO pion interactions have no  $O(a)$  corrections for any  $\omega_0$

$$\mathcal{L}_{\chi, LO} = \frac{f^2}{4} \text{Tr}(D_\mu \Sigma_{ph} D_\mu \Sigma_{ph}^\dagger) - \frac{f^2}{4} |\chi'| \text{Tr}(\Sigma_{ph} + \Sigma_{ph}^\dagger)$$



# NLO result: $O(a)$ improvement at $\omega_0 = \pi/2$

- express chiral Lagrangian in terms of  $\chi'$ :

$$\mathcal{L}_{\chi, \text{NLO}} = \text{continuum terms} + \tilde{W} \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\ - W \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) + O(a^2)$$

- Lagrangian is invariant under symmetry:

- $\pi \rightarrow -\pi, \omega_0 \rightarrow -\omega_0 \Rightarrow \Sigma \leftrightarrow \Sigma^\dagger, \chi' \leftrightarrow \chi'^\dagger$

which implies:

- $\text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma)$  and  $\text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi')$  are even in  $\pi$
- $\text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) = \cos \omega_0 \times (\text{even in } \pi) + \sin \omega_0 \times (\text{odd in } \pi)$

- for  $\omega_0 = \pi/2$ , physical vertices, with an even number of pions, receive no  $O(a)$  contributions
  - unphysical vertices with an odd number of pions are  $O(a)$
- $\Rightarrow$  **automatic  $O(a)$  improvement valid even if  $m_q \sim a\Lambda_{QCD}^2$  as long as use  $\omega_0$  and not  $\omega$**

# Recall: Kinematics of continuum tmQCD

Currents and densities:

$$A_\mu^j = \bar{\psi} \gamma_\mu \gamma_5 \tau_j \psi, \quad V_\mu^j = \bar{\psi} \gamma_\mu \tau_j \psi, \quad P^j = \bar{\psi} \gamma_5 (\tau_j / 2) \psi, \quad S^0 = \bar{\psi} \psi$$

Relation between operators in twisted and physical bases  
( $a = 1, 2$ ):

$$\begin{aligned} \hat{A}_\mu^a &= \cos \omega A_\mu^a + \epsilon^{3ab} \sin \omega V_\mu^b, & \hat{A}_\mu^3 &= A_\mu^3, \\ \hat{V}_\mu^a &= \cos \omega V_\mu^a + \epsilon^{3ab} \sin \omega A_\mu^b, & \hat{V}_\mu^3 &= V_\mu^3, \\ \hat{P}^3 &= \cos \omega P^3 + i \sin \omega S^0 / 2, & \hat{P}^a &= P^a, \\ \hat{S}^0 &= \cos \omega S^0 + 2i \sin \omega P^3 \end{aligned}$$

# Specific NLO results: twist angle

- How determine  $m'$  and thus  $\omega_0$ ?

(1) enforce  $\langle \hat{V}_\mu^2(x) \hat{P}^1(y) \rangle = 0$  implying

$$\tan \omega_A \equiv \frac{\langle V_\mu^2(x) P^1(y) \rangle}{\langle A_\mu^1(x) P^1(y) \rangle}$$

(2) enforce  $\langle \hat{S}^0(x) \hat{A}_\mu^3(y) \rangle = 0$  implying

$$\tan \omega_P \equiv \frac{i \langle S^0(x) A_\mu^3(y) \rangle}{2 \langle P^3(x) A_\mu^3(y) \rangle}$$

- result:  $\omega_0$  determined to  $O(\alpha)$  accuracy

$$\omega_0 = \omega_A + \frac{16\hat{a}s}{f^2} (W + W_{10}/4 + 2\hat{a}cW'/(2B_0m_q))$$

$$\omega_P = \omega_A + \frac{4\hat{a}s(4W + W_{10})}{f^2}$$

with  $c = \cos \omega_A$  and  $s = \sin \omega_A$

# Required accuracy for twist angle?

- $O(a)$  ambiguity in  $\omega$  is inevitable due to discretization errors
- ambiguity does not impact automatic  $O(a)$  improvement

$$\begin{aligned} Q_{\text{lat}} &= Q_{\text{cont}} [1 + a \cos \omega + O(a^2)] \\ \delta Q_{\text{lat}} &= Q_{\text{cont}} a \delta(\cos \omega) + O(a^2) \\ &= -Q_{\text{cont}} a \sin \omega \delta \omega + O(a^2) \\ &= O(a^2) \end{aligned}$$

⇒ can set either  $\omega_A = \pi/2$  or  $\omega_P = \pi/2$

- we propose  $\omega_A = \pi/2$  as canonical choice since easier to implement in simulations

# Specific NLO results: pion masses

- Charged pion mass is automatically improved:  
result agrees with [Scorzato]

$$m_{\pi_{\pm}}^2 = |\chi'| + \frac{16}{f^2} \left[ |\chi'|^2 (2L_{68} - L_{45}) + |\chi'| \hat{a} c (2W - \widetilde{W}) + 2\hat{a}^2 c^2 W' \right] + \text{cont. 1-loop} + \dots$$

- Pion isospin splitting is  $O(a^2)$  and maximal for  $\omega = \pi/2$ :

$$\begin{aligned} m_{\pi_3}^2 - m_{\pi_{1,2}}^2 &= -\frac{32}{f^2} \hat{a}^2 s^2 W' + O(a^3) \\ &= -W' \frac{32}{f^2} \frac{\hat{a}^2 \mu^2}{m'^2 + \mu^2} + O(a^3) \end{aligned}$$

- Harder to calculate numerically as requires quark-disconnected contractions
- Measures constant  $W'$

# Specific NLO results: matrix elements

- Pion decay constant agrees with [Münster & Schmidt]

$$f_A = f \left\{ 1 + \frac{4}{f^2} \left[ 2|\chi'| L_{45} + \hat{a}c(2\tilde{W} + W_{10}) \right] + \text{cont. 1-loop} \right\}$$

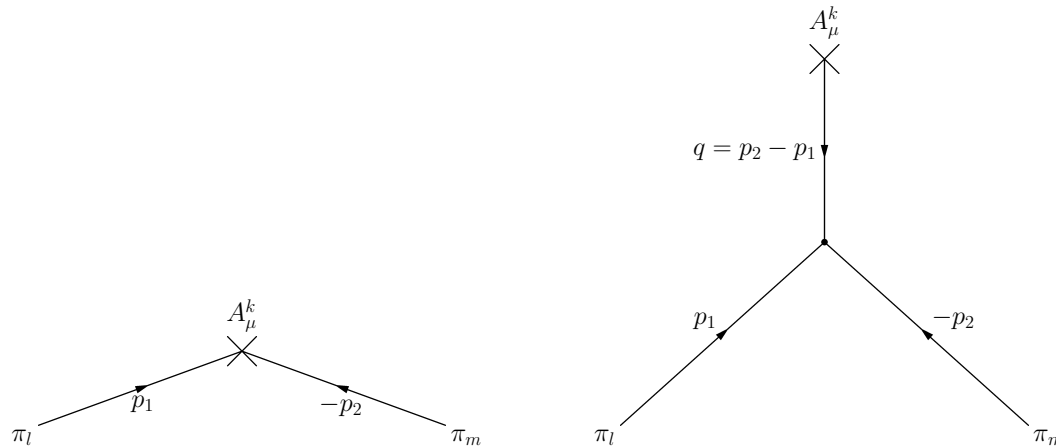
- flavor breaking only at NNLO
- Results for  $\langle 0|P|\pi\rangle$ , scalar and vector form factors, have similar form showing automatic  $O(a)$  improvement and no flavor breaking
- can measure physical condensate using  $P^3$

$$\langle 2iP^3 \rangle = -2f^2 B_0 s \left\{ 1 + \frac{4}{f^2} \left[ |\chi'| (8L_{68} + H_2) + \hat{a}c(4W + W_{10}) \right] + 1\text{-loop} \right\}$$

# Parity violating matrix elements

Axial and pseudoscalar form factors of pion non-vanishing, e.g.

$$\langle \pi_a | \hat{A}_\mu^a | \pi_3 \rangle, \langle \pi_a | \hat{A}_\mu^3 | \pi_a \rangle, \langle \pi_3 | \hat{A}_\mu^3 | \pi_3 \rangle,$$



Example of results:

$$\langle \pi_a(p_2) | \hat{P}^3 | \pi_a(p_1) \rangle = \frac{16 \hat{a} s i B_0}{f^2} \left[ \frac{-W_{10}}{4} + W - \widetilde{W} + \frac{2 \hat{a} c W'}{q^2 + m_{\pi_3}^2} + \frac{(\widetilde{W}/2 - W) q^2}{q^2 + m_{\pi_3}^2} \right]$$

- present at maximal twisting  $s = 1, c = 0$
- use to determine all  $W$ 's and then to test  $\text{tm}_\chi\text{PT}$  at NLO

# Summary for $m_q \sim a\Lambda_{QCD}^2$

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- Predicted functional forms for pionic quantities for all  $\mu, m'$
- Can determine maximal twisting non-perturbatively using  $\omega_A = \pi/2$  or  $\omega_P = \pi/2$  (or by maximizing pion mass splitting)
  - automatically includes  $O(a)$  shift in  $m_c$
  - $O(a)$  ambiguity in  $\omega$  cannot be avoided
- Automatic  $O(a)$  improvement at maximal twist holds in GSM regime
- Parity-flavor violating quantities ( $\omega_A - \omega_P$ , axial and pseudoscalar form factors) are  $O(a)$ 
  - provide measure of discretization errors, i.e. size of  $W$ 's
  - provide tests of tm $\chi$ PT at NLO
  - can correct *a posteriori*  $O(a)$  errors in untwisted simulations
- Flavor breaking in physical quantities occurs at  $O(a^2)$ 
  - only example in NLO calculation is pion mass splitting



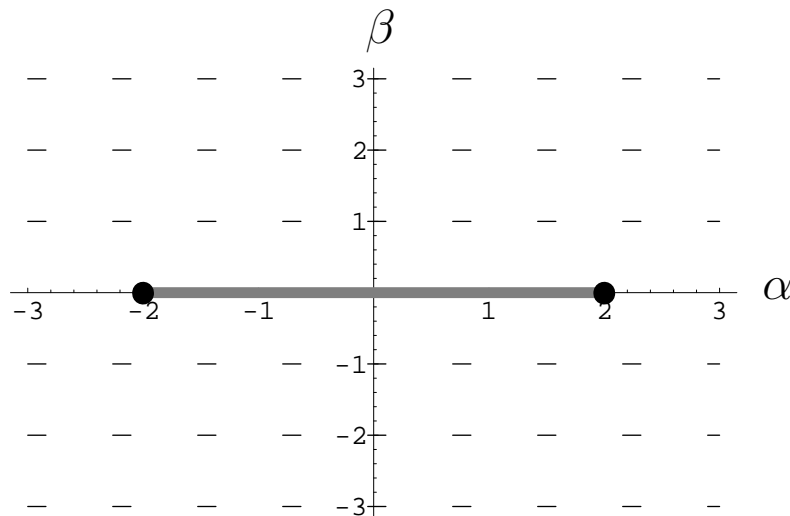
# Results for Aoki regime

- Work to LO in power counting  $m_q \sim a^2 \Lambda_{QCD}^3$
- Lagrangian collapses to:

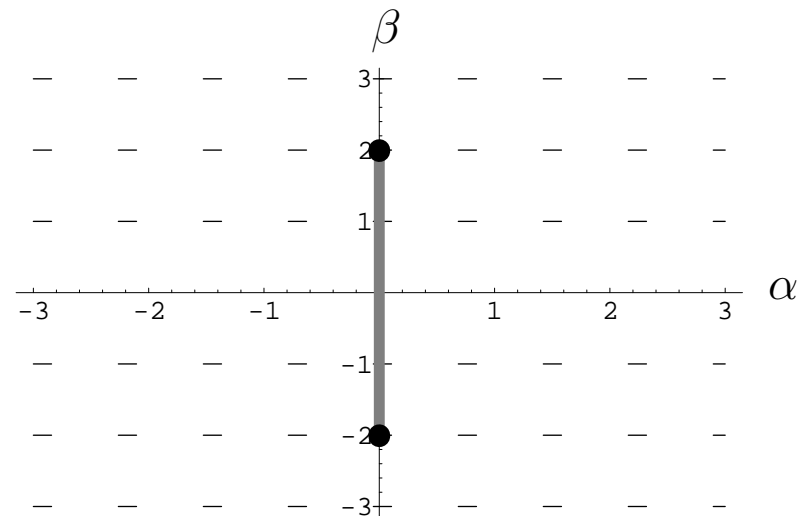
$$\begin{aligned} \mathcal{L}_\chi = & \frac{f^2}{4} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f^2}{4} \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') - W' [\text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A})]^2 \\ & + \tilde{W} \text{Tr}(D_\mu \Sigma^\dagger D_\mu \Sigma) \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) - W \text{Tr}(\chi'^\dagger \Sigma + \Sigma^\dagger \chi') \text{Tr}(\hat{A}^\dagger \Sigma + \Sigma^\dagger \hat{A}) \\ & + W_{10} \text{Tr}(D_\mu \hat{A}^\dagger D_\mu \Sigma + D_\mu \Sigma^\dagger D_\mu \hat{A}) + O(a^3) \end{aligned}$$

- Competition between  $m_q$  and  $a^2$  terms leads to non-trivial phase structure [Aoki, Creutz, SRS & Singleton, Münster, Scorzato, SRS & Wu]
- Phase structure depends on sign of  $W'$  (which also determines the sign of pion mass splitting [Scorzato] )
- Can extend calculations from GSM regime into Aoki regime

# Possible phase diagrams in Aoki regime



(a) Phase diagram for  $c_2 > 0$



(b) Phase diagram for  $c_2 < 0$

$$c_2 = -16W'\hat{a}^2, \quad \alpha = 2B_0f^2m'/|c_2|, \quad \beta = 2B_0f^2\mu/|c_2|$$

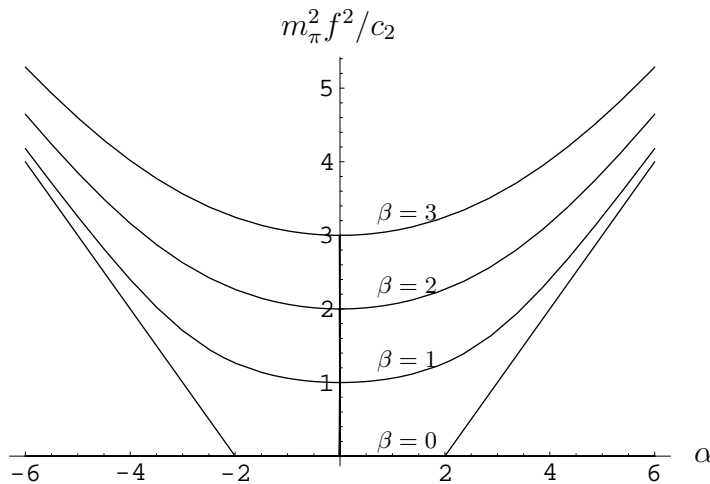
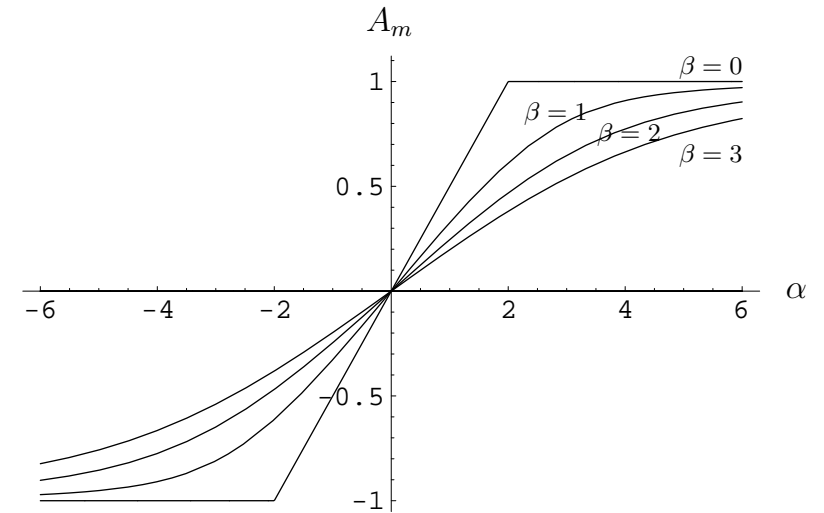
- Solid lines are first-order phase transitions with second-order endpoints

# $W' < 0$ : Aoki phase

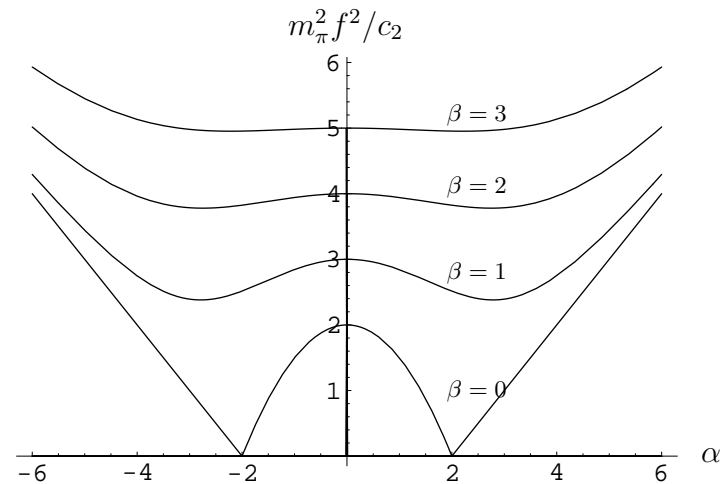
- Condensate:

$$\langle 0|\Sigma|0\rangle = A_m + iB_m\tau_3$$

- Aoki phase washed out for  $\mu \propto \beta \neq 0$
- Note  $A_m = 0$  for  $\alpha = m' = 0$



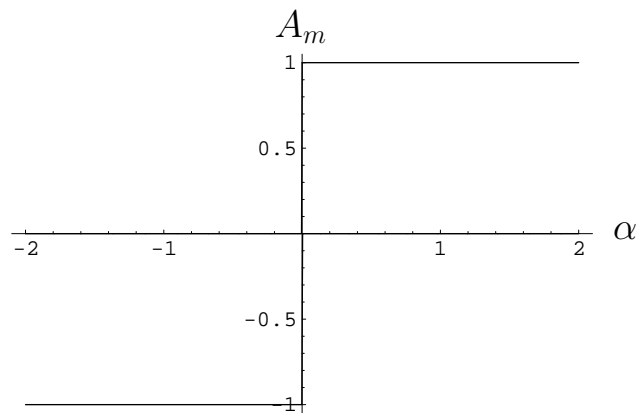
(a) Mass of  $\pi_1$  and  $\pi_2$



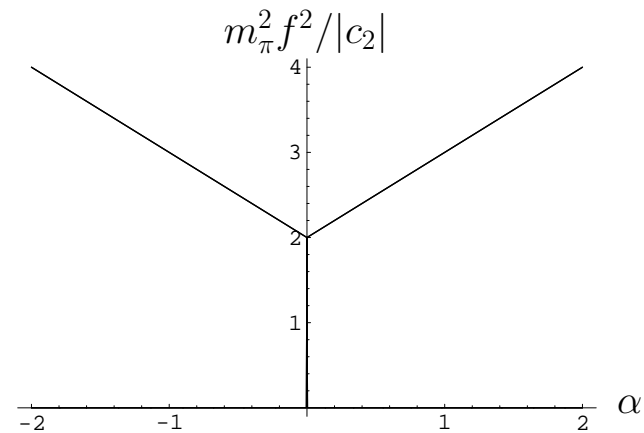
(b) Mass of  $\pi_3$

# $W' > 0$ : no Aoki phase

Along Wilson axis:

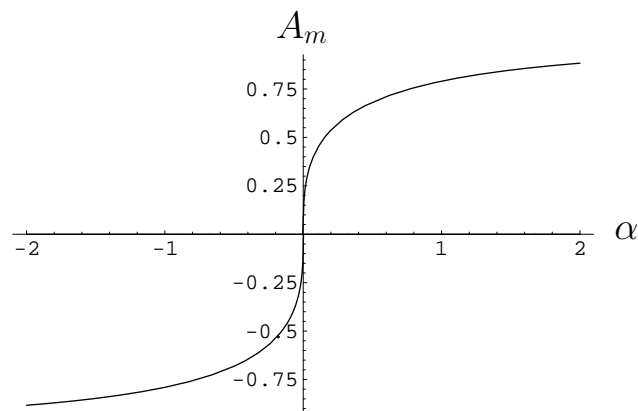


(a) Global minimum,  $\beta = 0$

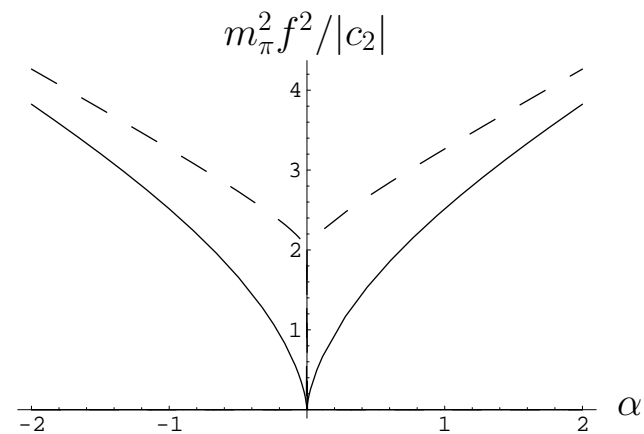


(b) Pion masses,  $\beta = 0$

At top of phase transition: **dashed: charged; solid: neutral**



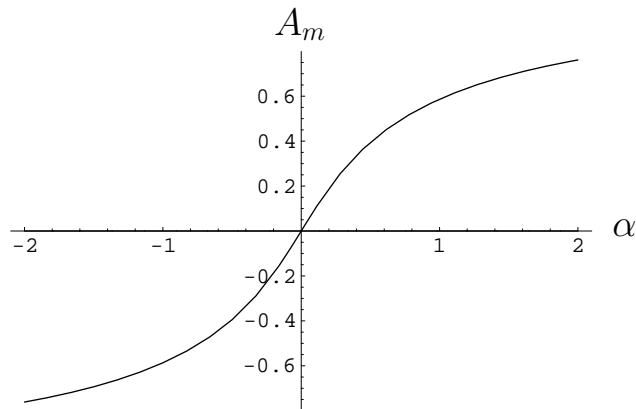
(e) Global minimum,  $\beta = 2$



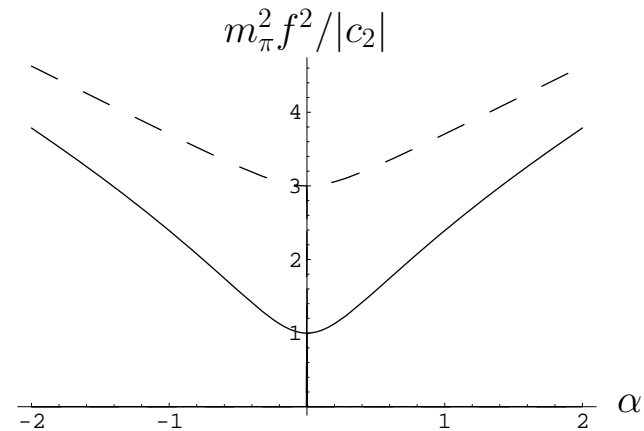
(f) Pion masses,  $\beta = 2$

# More on $W' > 0$

Above phase transition: **dashed: charged; solid: neutral**



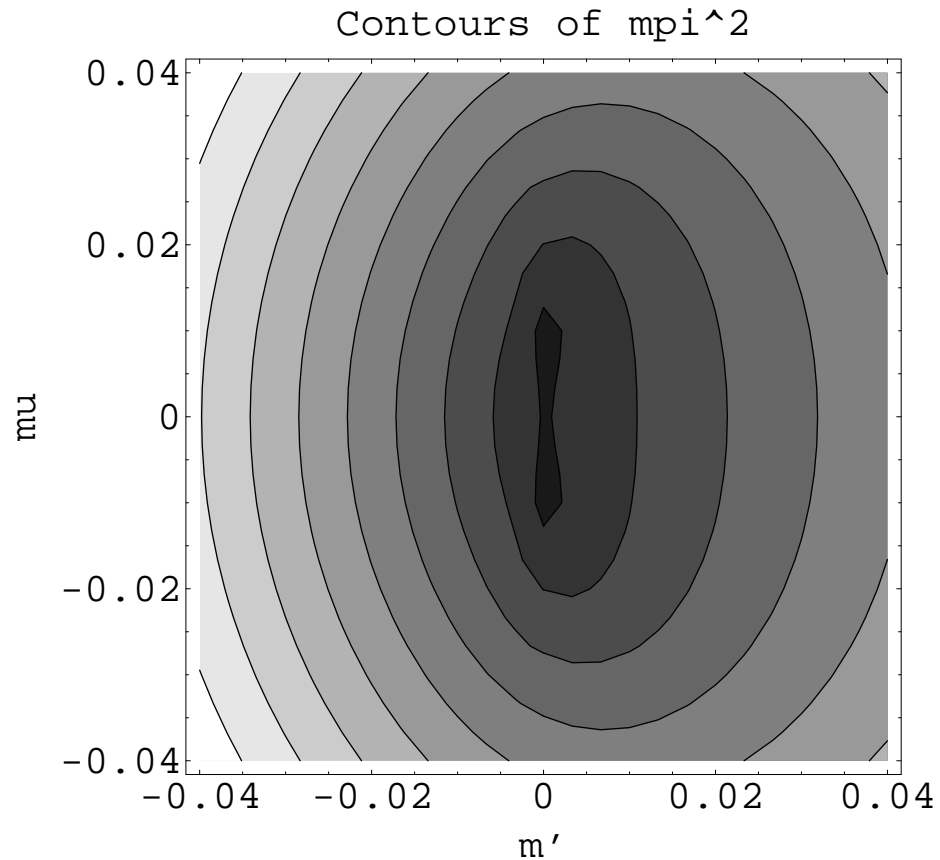
(g) Global minimum,  $\beta = 3$



(h) Pion masses,  $\beta = 3$

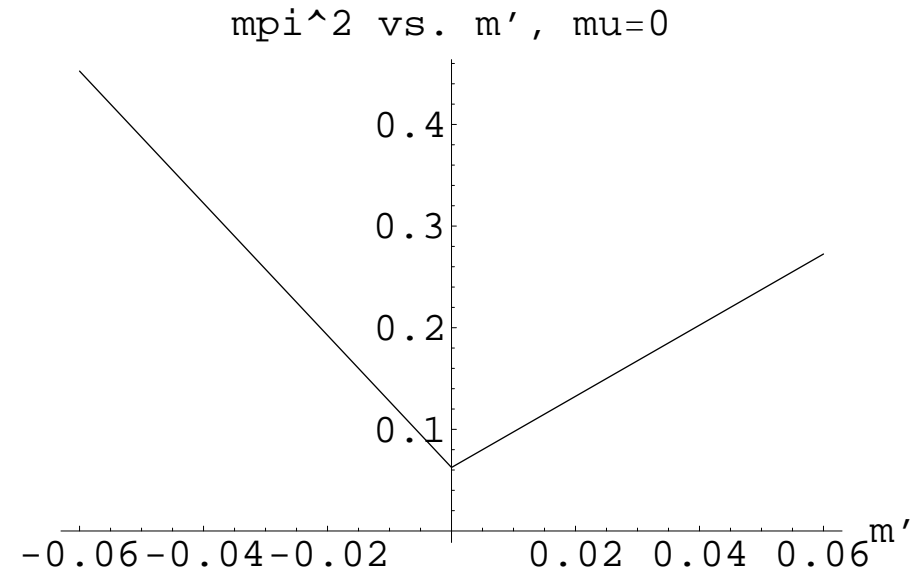
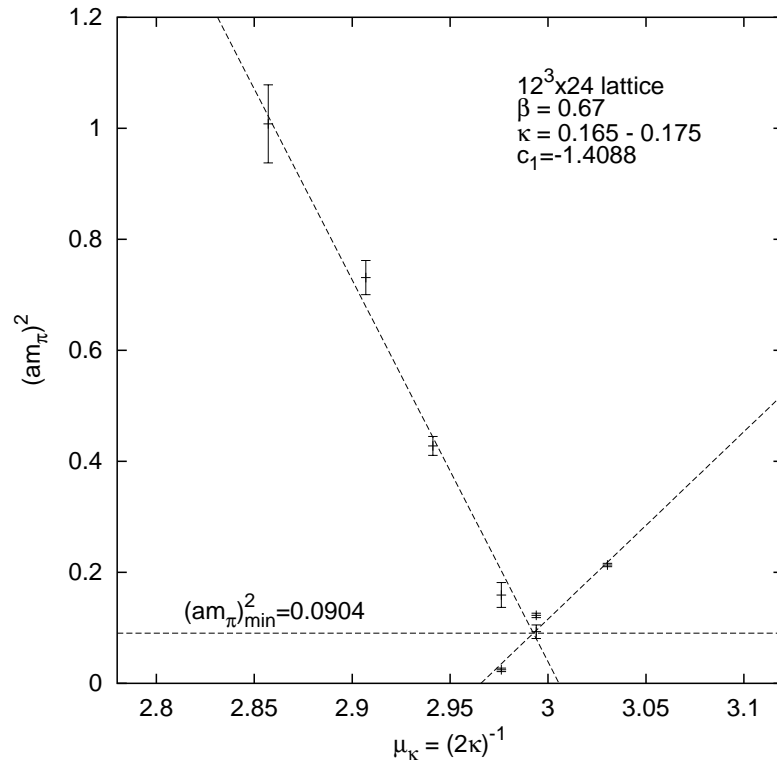
- Can use minimum of pion masses as an alternative for determining where  $m' = 0$
  - Away from transition, condensate has  $A_m = 0$  for maximal twisting, i.e. lies along direction of quark mass as in continuum
- ⇒ Automatic  $O(a)$  improvement at maximal twist still holds in Aoki regime away from phase transitions [Aoki & Bär]

# Predictions from $tm\chi PT$



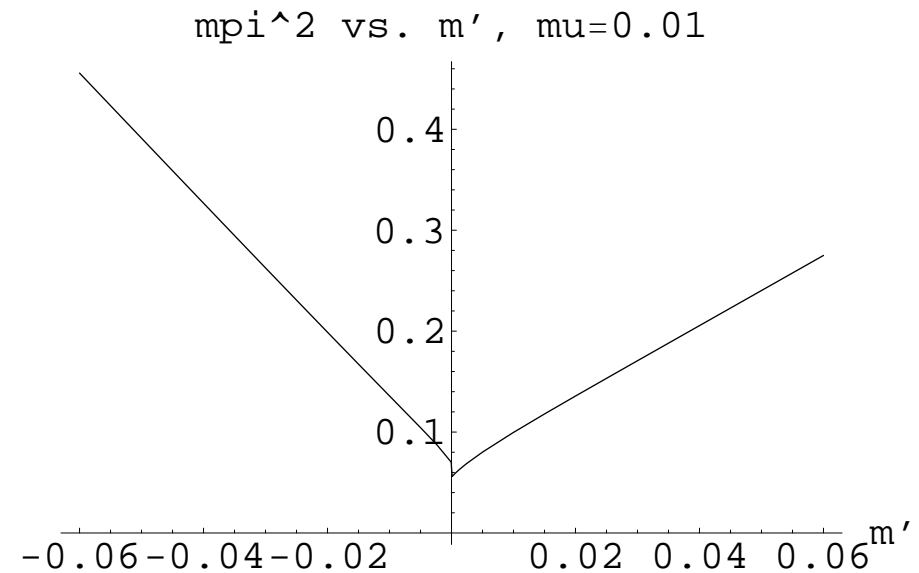
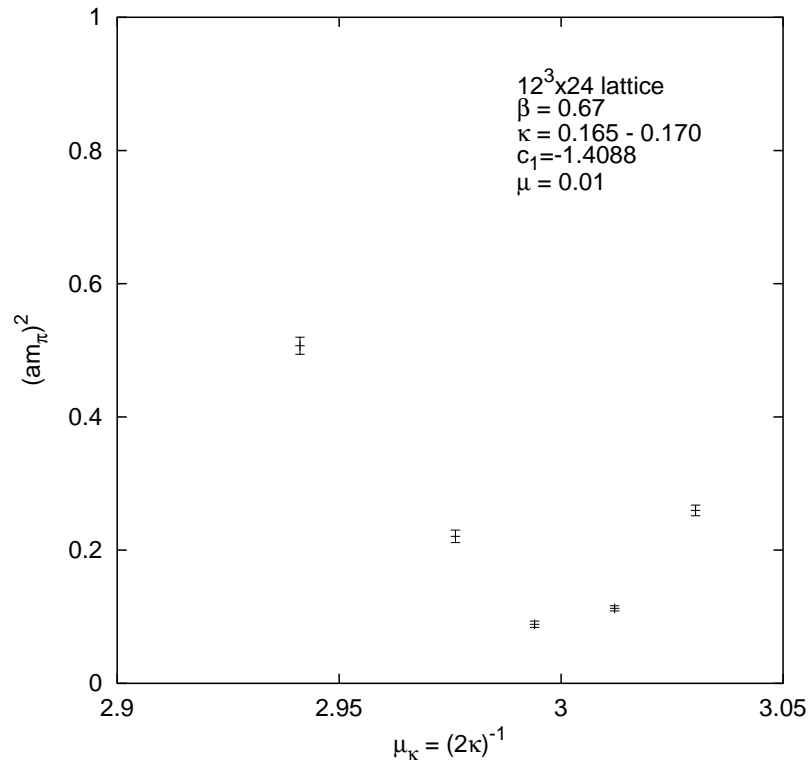
Contour plot of charged  $m_{\pi^2}$  from  $tm\chi PT$  with parameters roughly tuned to match those of hep-lat/0410031, Farchioni *et al.*

# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



- Qualitative comparison only
- Difference in slopes for positive and negative  $m'$  caused by a 30%  $\hat{a}(2W - \tilde{W}) \cos(\omega_A)$  correction

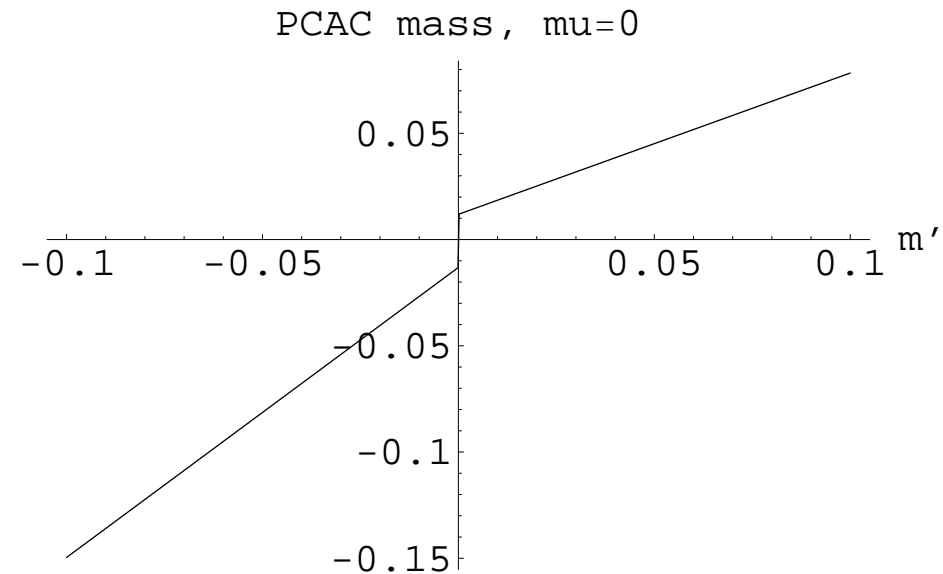
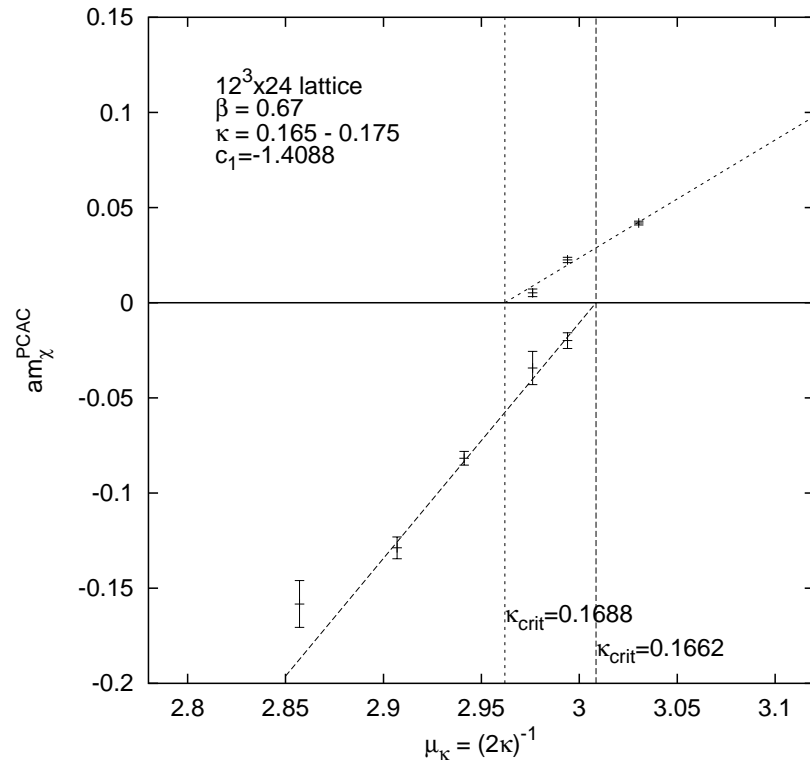
# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



- Qualitative comparison only
- Difference in slopes for positive and negative  $m'$  caused by a 30%  $\hat{a}(2W - \tilde{W}) \cos(\omega_A)$  correction

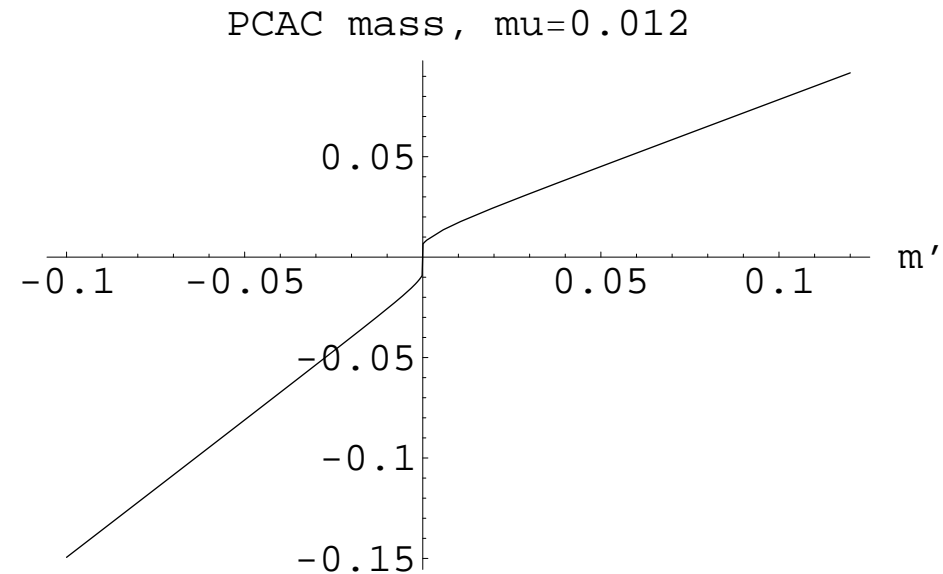
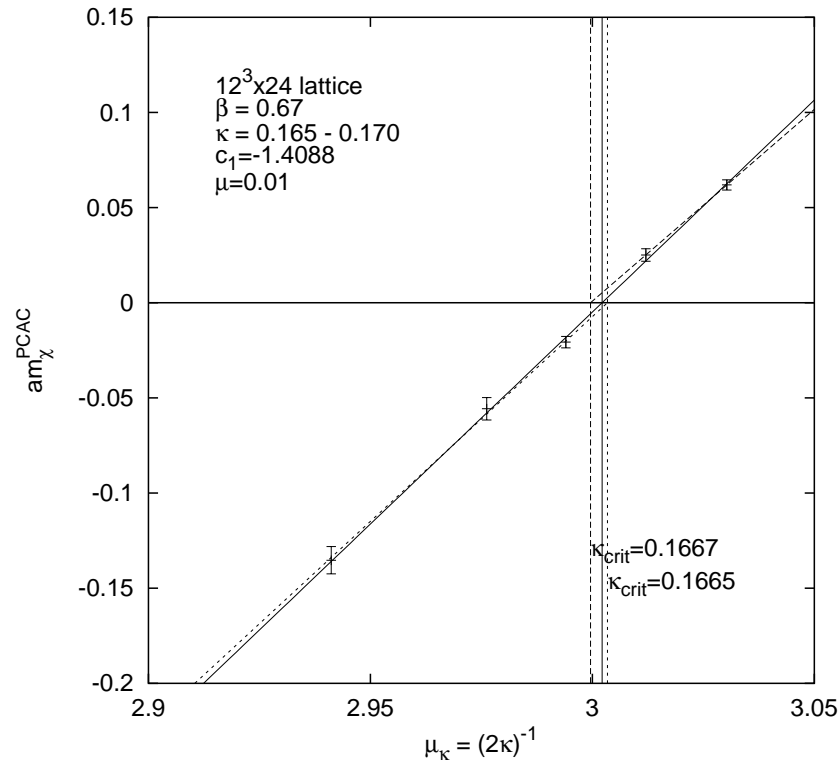


# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



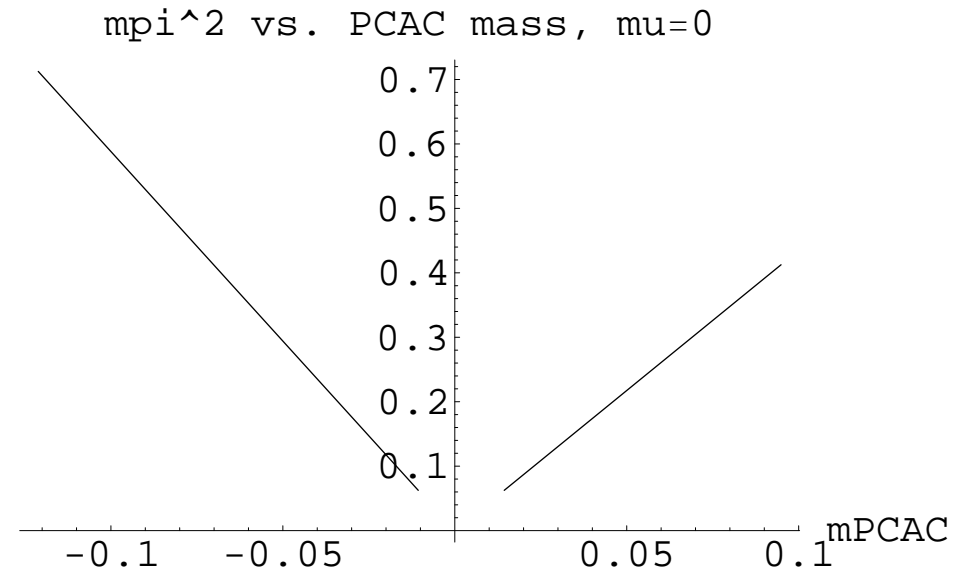
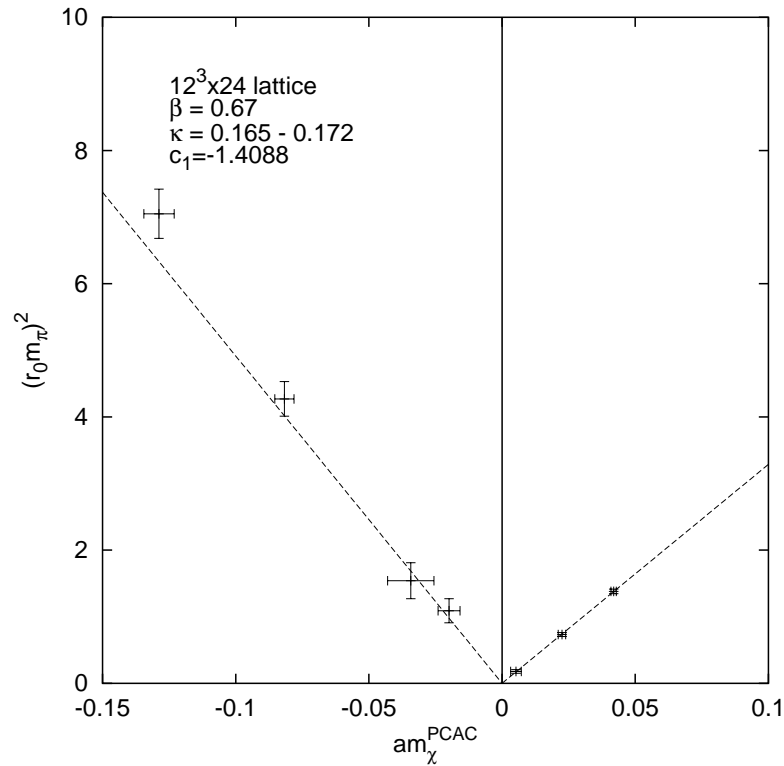
- Qualitative comparison only
- Difference in slopes for positive and negative  $m'$  caused by  $\hat{a} \cos(\omega_A)$  correction

# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



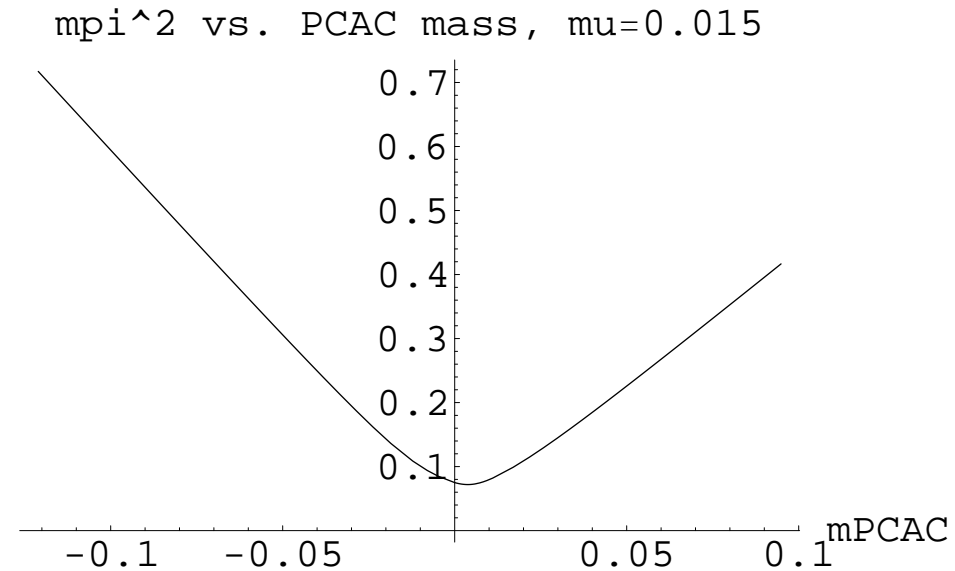
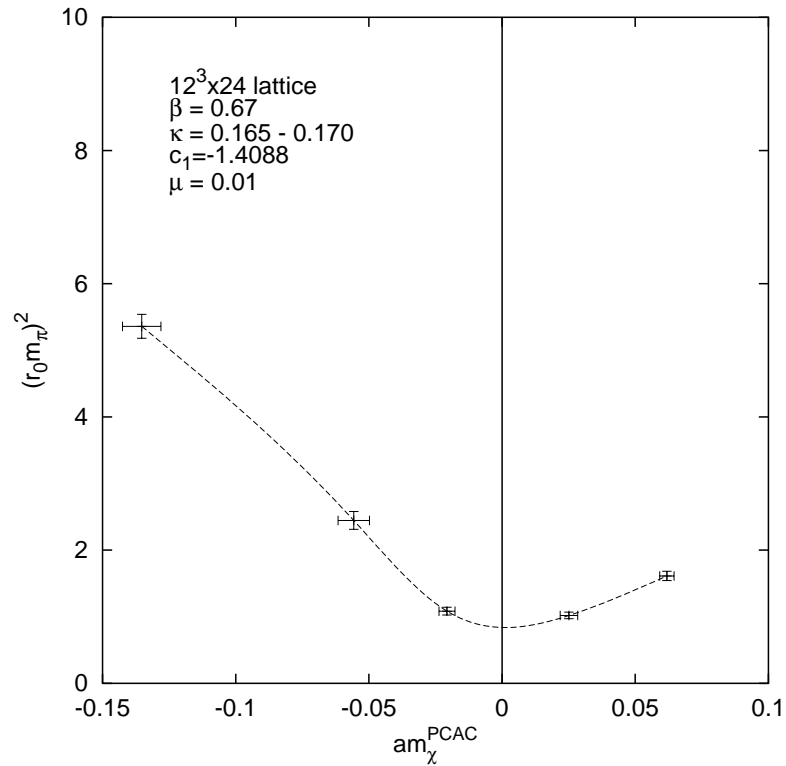
- $\chi$ PT does *not* explain the change in relative slopes as  $\mu$  increases

# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



- Data goes to lighter pion mass because of metastability

# Comparing $\chi$ PT with [Farchioni et al, hep-lat/0410031]



- $\chi$ PT curve is above phase boundary so no minimum  $m_{PCAC}$

# Summary and outlook

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- Automatic  $O(a)$  improvement works for  $m_q \geq c' a^2 \Lambda_{QCD}^3$ 
  - But essential to use an appropriate definition of twisting angle
- Parity-flavor violating quantities provide interesting window on theory, and will allow test of our understanding
- Flavor violation in most parity conserving quantities requires NNLO calculation (underway)
- Many interesting quantities have disconnected contractions so hard to calculate
  - Use partially quenched tm  $\chi$ PT to separate connected and disconnected contractions?
- tmLQCD is a potential competitor to improved staggered fermions matching its advantages but without its major drawback and merits intensive study