Phase Structure of Wilson and twisted-mass fermions in the presence of isospin breaking

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Based on Derek Horkel + SS
[1409.2548, 1505.02218, 1507.03653]

"Phase diagram of nondegenerate twisted mass fermions"

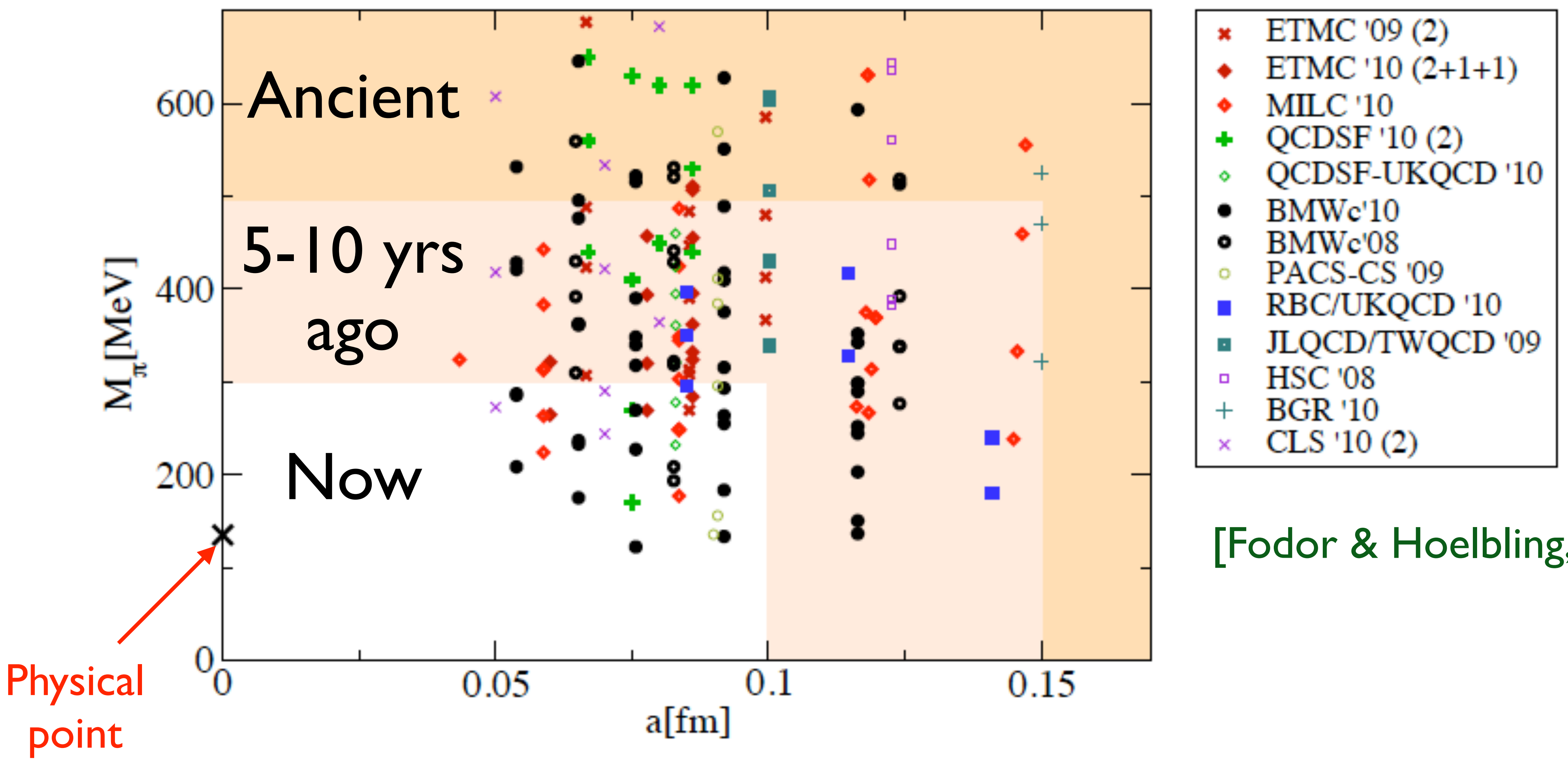
"Impact of electromagnetism on phase structure for Wilson and twisted-mass fermions including isospin breaking"

"Phase structure with nonzero Θ_{QCD} and twisted mass fermions"

Outline

- Introduction
- ChPT for Wilson and twisted-mass fermions
- Phase structure with isospin breaking
- Tuning to maximal twist with isospin breaking

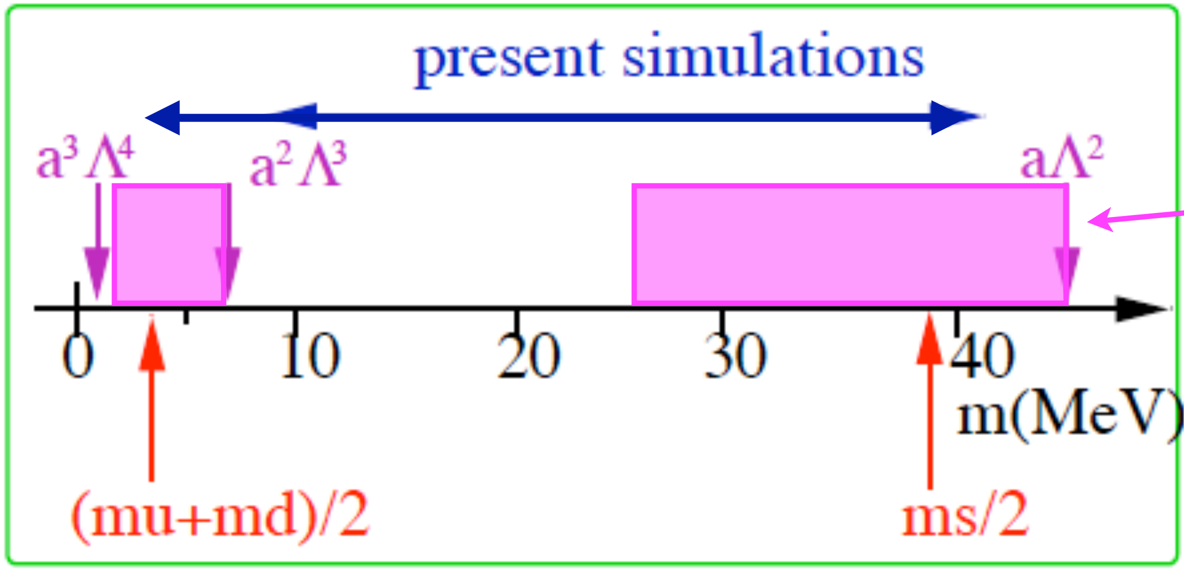
Era of physical quark masses



[Fodor & Hoelbling, RMP12]

- Present frontier is the inclusion of isospin breaking
  - $m_u \neq m_d$ and $\alpha_{EM} \neq 0$

Importance of discretization errors



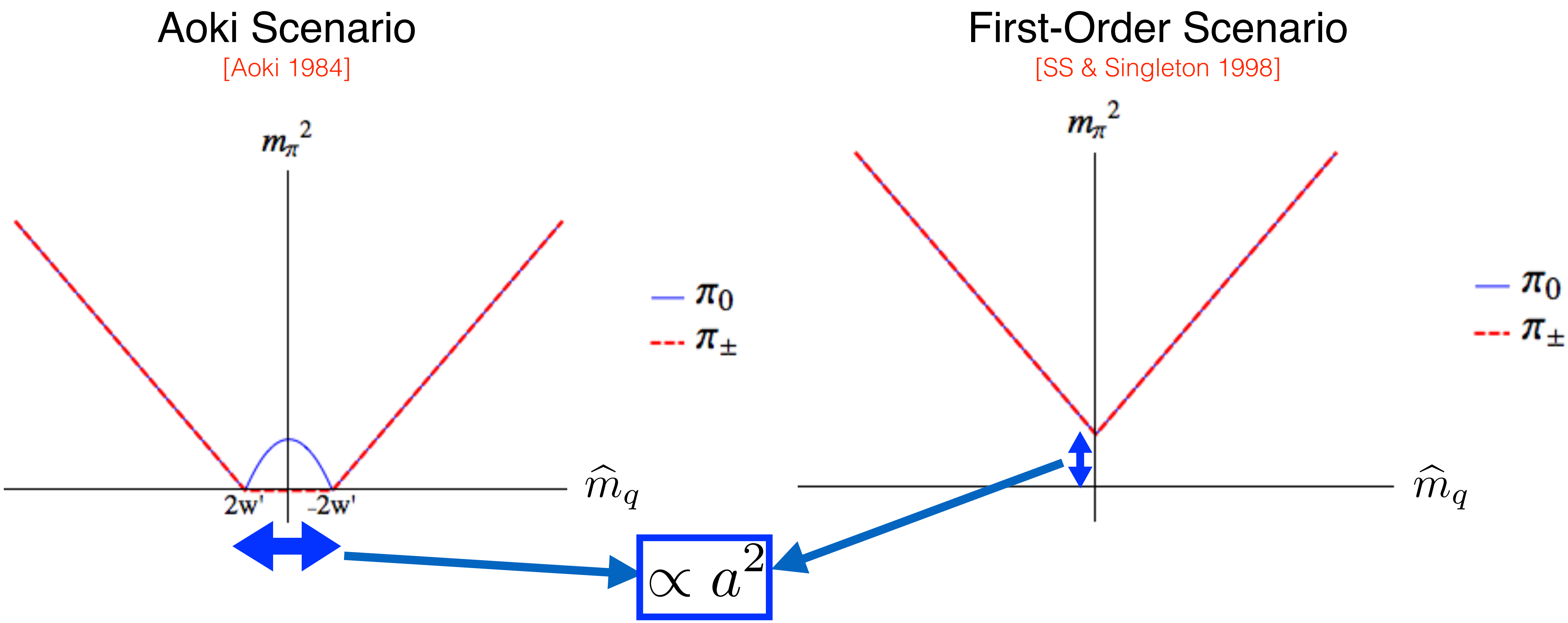
Using a=0.05-0.1fm & Λ_{QCD}=300 MeV

- With physical light quark masses (light ⇒ u & d)
  - $m_{u,d} \approx a^2\Lambda^3 \ll a\,\Lambda^2$
  - O(a) effects must be removed (improved actions) and O(a^2) effects understood

Importance of discretization errors

- Discretization errors play a special role for Wilson & twisted mass fermions
- They lead to chiral symmetry breaking and thus compete with the explicit chiral symmetry from quark masses
- Can lead to unphysical phases that one should learn about (and then avoid!)
    - E.g. Aoki phase (spontaneous flavor and parity breaking)

Unphysical phases ($m_u = m_d$)



- New phases introduced by the lattice have long been understood for degenerate quark masses without electromagnetism
- The phase structure is understood using chiral perturbation theory (ChPT) for both Wilson and twisted mass fermions
- The phase diagram must be reinvestigated with isospin breaking

This really happens!

[Farchioni et al., 05]

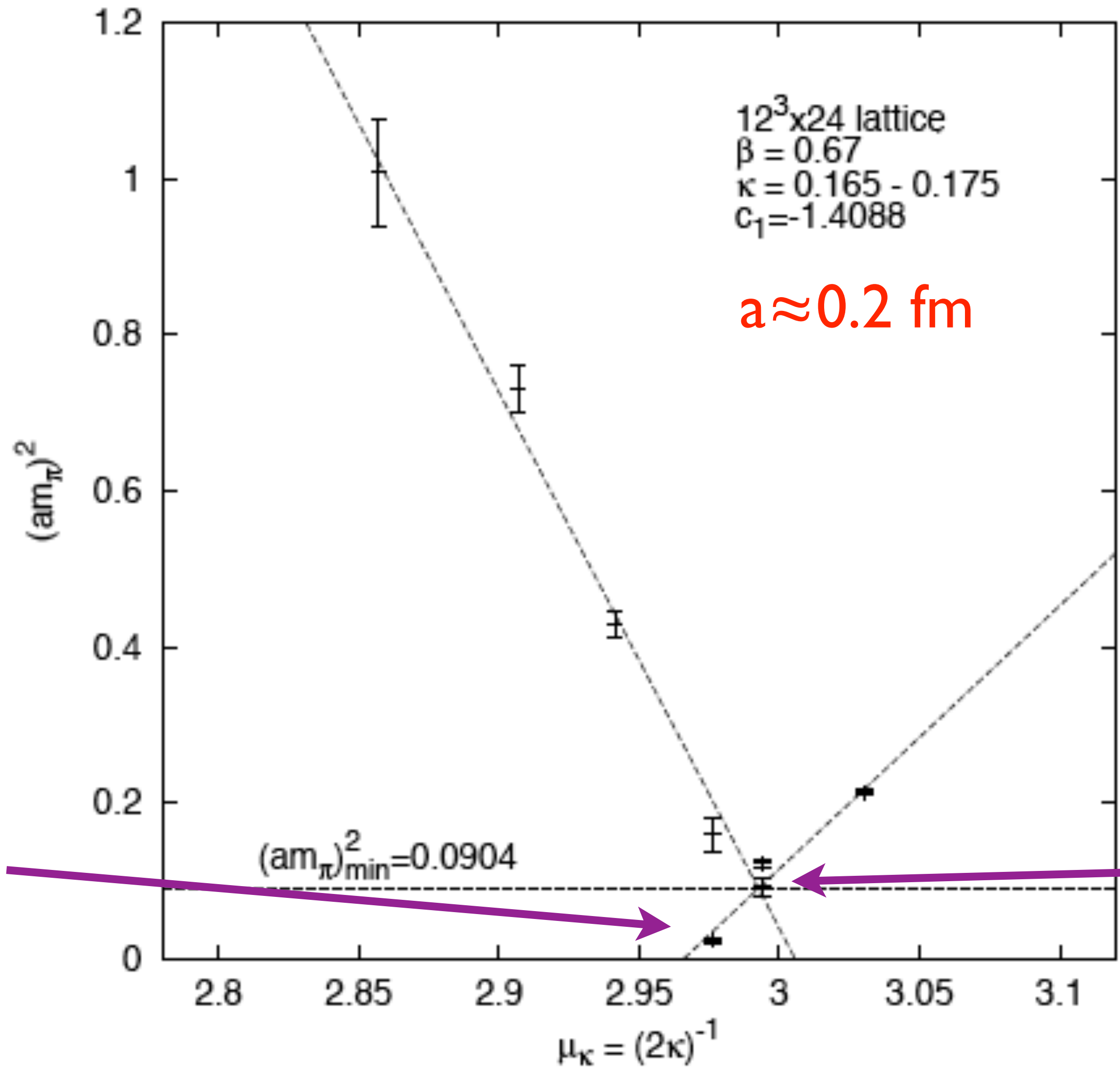


Figure 9. Unquenched results for $(am_\pi)^2$ as a function of $(2\kappa)^{-1} = m_0 + 4$ for $\mu = 0$ and with $a^{-1} \approx 0.2$ fm[60]. Straight lines are to guide the eye.

Evidence for first-order nature of transition from presence of "super cooled" phase

First-order scenario with minimum pion mass

Caveat: LO WChPT may not apply for such a coarse lattice

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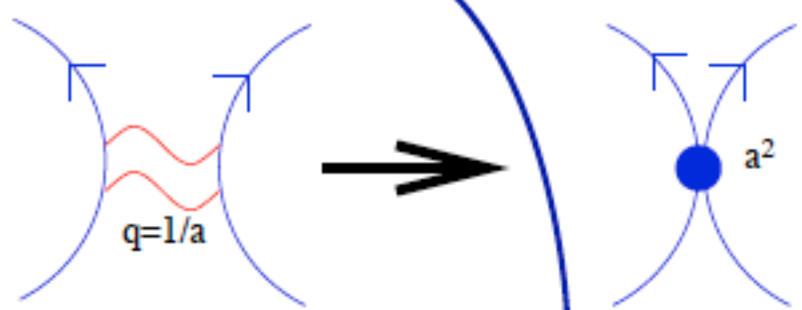
General strategy

Proceed in two steps: [Sharpe & Singleton]

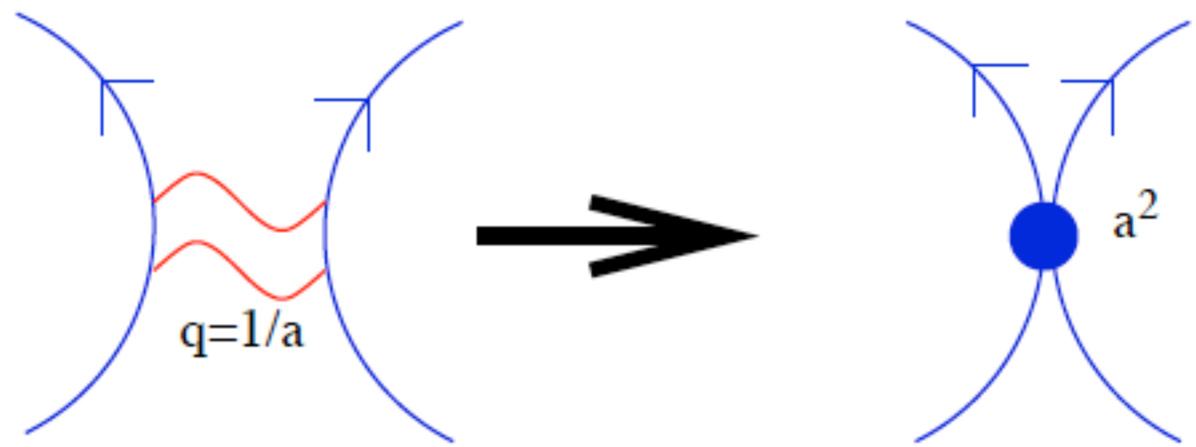
Lattice Lagrangian:
Wilson, tm, staggered



Continuum effective Lagrangian:
continuum quark-level theory including explicit nonzero a effects [Symanzik]

Chiral Lagrangian:
continuum χPT plus effects of additional operators induced by discretization

Symanzik EFT ("SET")



- Integrate out high-momentum quarks and gluons ($p \sim 1/a$), obtain a local EFT describing low-momentum modes ($p \ll 1/a$)

$$\mathcal{L}_{\rm eff} = \mathcal{L}_{\rm tmQCD} + a\mathcal{L}^{(5)} + a^2\mathcal{L}^{(6)} + \ldots$$

absent for improved action

  - Regularize with continuum regulator or finer lattice
  - Factors of a explicit
  - "a" means $\sim a(1 + g[a]^2 \ln a + \ldots)$
  - $\mathcal{L}^{(5,6,\ldots)}$ contain all operators allowed by *lattice symmetries*

- $\mathcal{L}_{\rm eff}$ gives discretization errors to **all** correlation functions
  - Holds to all orders in PT (where can calculate $\mathcal{L}^{(5,6,\ldots)}$) [Symanzik]
  - Demonstrates validity of EFT directly in Euclidean space

SET for Wilson & twisted mass fermions

$$\mathcal{L}^{(5)}_{\rm NLO} \sim \bar\psi i\sigma_{\mu\nu}F_{\mu\nu}\psi \longleftarrow \boxed{\text{absent for improved action}}$$

$$\begin{aligned}\mathcal{L}^{(6)}_{\rm NLO} \sim\ & \mathrm{Tr}(D_\mu F_{\rho\sigma} D_\mu F_{\rho\sigma}) + \mathrm{Tr}(D_\mu F_{\mu\sigma} D_\rho F_{\rho\sigma}) \\ & + \bar\psi D_\mu \not{D} D_\mu \gamma_\mu \psi + \cdots + (\bar\psi\psi)^2 + (\bar\psi\gamma_\mu\psi)^2 + \dots \\ & + \underbrace{\mathrm{Tr}(D_\mu F_{\mu\sigma} D_\mu F_{\mu\sigma}) + \bar\psi D_\mu^3 \gamma_\mu \psi}_{\text{Lorentz violating}}\end{aligned}$$

[Lüscher & Weisz 85; Sheikholeslami & Wohlert 85; Lüscher, Sint, Sommer & Weisz 96; SS & Wu 05]

- Some of the fermionic terms in the SET break chiral symmetry in the same way as the quark mass term

$$\mathcal{L}_{\rm QCD} \supset \bar\psi M \psi = \overline{\psi_L} M \psi_R + \overline{\psi_R} M \psi_L$$

violates (global) transformation

$$\psi_{L,R} \to U_{L,R}\psi_{L,R} \qquad \overline{\psi}_{L,R} \to \overline{\psi}_{L,R} U^\dagger_{L,R} \qquad U_{L,R} \in SU(2)$$

Chiral perturbation theory

- ChPT describes the low energy properties of QCD; it is valid because spontaneous chiral symmetry breaking leads to a mass gap
- Pseudo-Goldstone bosons collected into a field $\Sigma \in SU(2)$

$$\Sigma = \langle\Sigma\rangle e^{2i\pi/f} \to U_L \Sigma U_R^\dagger \qquad \pi = \begin{pmatrix} \frac{\pi^0}{2} & \frac{\pi^+}{\sqrt{2}} \\ \frac{\pi^-}{\sqrt{2}} & -\frac{\pi^0}{2} \end{pmatrix}$$

- The effective theory is built by writing down the most general Lagrangian obeying the symmetries of QCD, treating the quark mass as a spurion
- At leading order (the order we will largely work today):

$$\mathcal{L}_{\chi LO} = \frac{f^2}{4} \mathrm{tr}(\partial_\mu \Sigma \partial_\mu \Sigma^\dagger) - \frac{B_0 f^2}{2} \mathrm{tr}(M\Sigma^\dagger + M^\dagger \Sigma))$$

power counting $\qquad \mathcal{O}(p^2 \sim B_0 m_q)$

low-energy coefficients (LECs) $\qquad f, B_0 \sim \Lambda_{QCD}$

Discretization effects in ChPT

- Mapping $\mathcal{L}^{(6)}$ into the chiral Lagrangian, the new term is

$$-W'\left(\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)\right)^2$$

A $\propto$ a**1**

New LEC associated with discretization errors
Depends on choice of action; sign unknown

- This term is leading order in the power counting appropriate to current simulations

$$p^2 \sim m \sim a^2$$

- Total LO chiral Lagrangian for Wilson and twisted mass fermions (WχPT)

$$\mathcal{L}_{\chi LO} = \frac{f^2}{4}\mathrm{tr}(\partial_\mu\Sigma\partial_\mu\Sigma^\dagger) - \frac{B_0 f^2}{2}\mathrm{tr}(M\Sigma^\dagger + M^\dagger\Sigma)) \; -W'\left(\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)\right)^2$$

twisted mass only affects M

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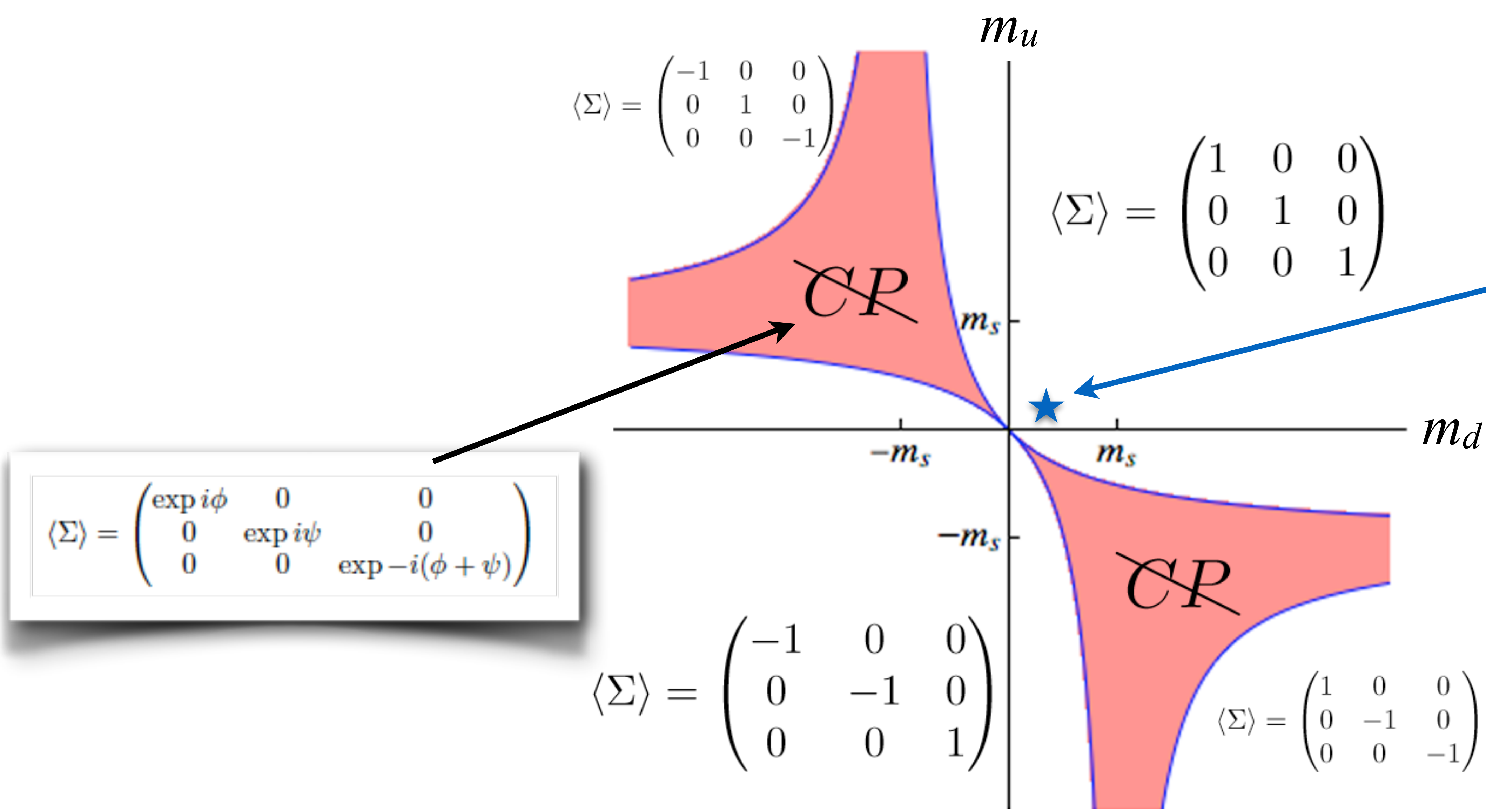
Unphysical phase in continuum

What happens to this phase at nonzero lattice spacing?
What is the relation to the Aoki phase?
What is the impact of EM?
What is the relevance for simulations?

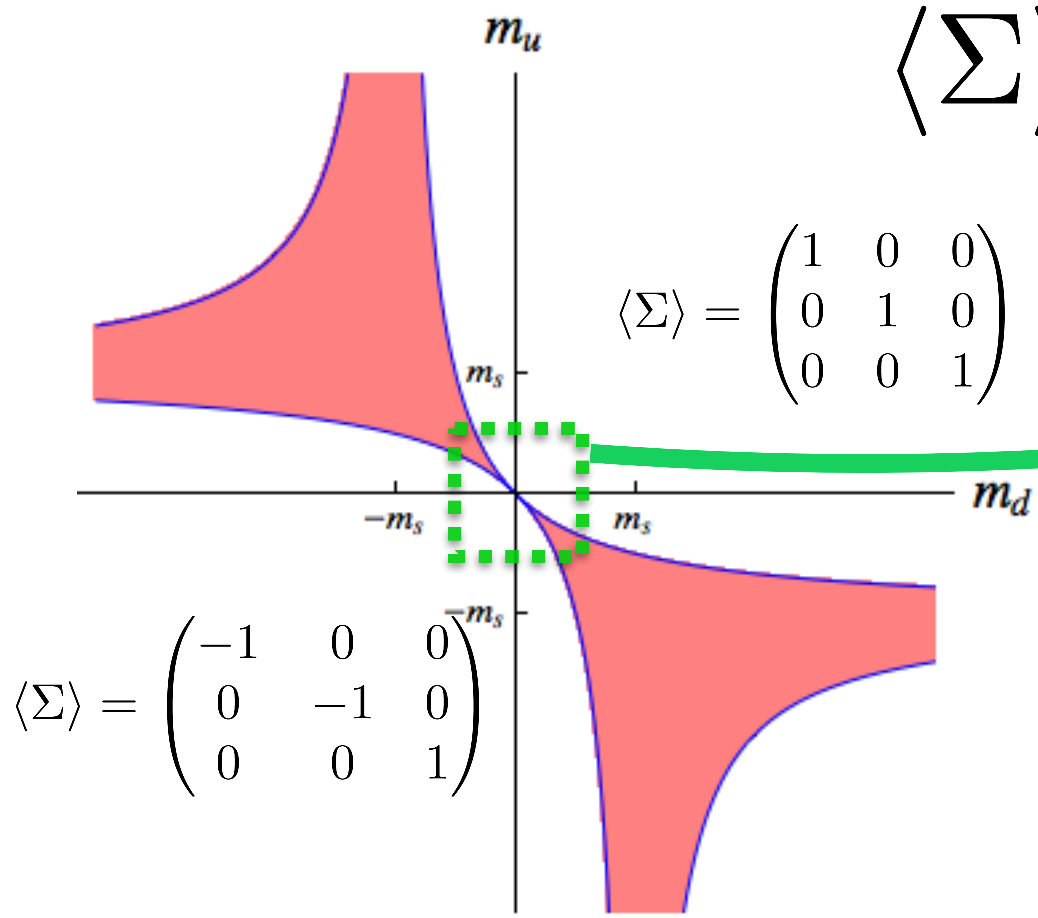


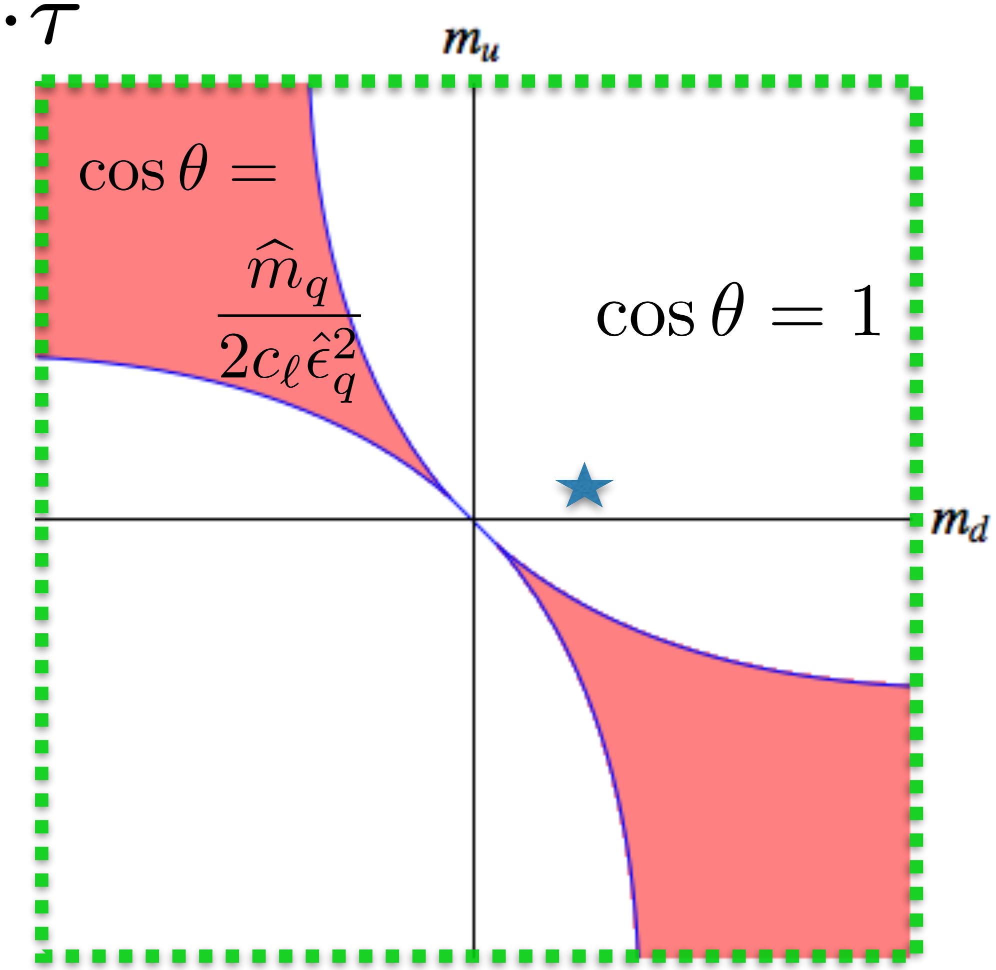
Reproduce Dashen-Creutz phase in SU(2) ChPT

- Needed to study twisted-mass fermions
- Requires one NLO term (arising from integrating out s quark)

$$\frac{\ell_7 B_0^2}{16}\left[\mathrm{tr}(M\Sigma^\dagger - M^\dagger\Sigma)\right]^2 \qquad \ell_7 = \frac{f^2}{8B_0 m_s}$$ [Gasser & Leutwyler 84]

$$\langle\Sigma\rangle = e^{i\theta\hat{n}\cdot\vec{\tau}}$$





$m_u = -m_d$ case studied by [Smilga 99]

Modified power counting

$$\mathcal{L}_{\chi LO} = \frac{f^2}{4}\,\mathrm{tr}(\partial_\mu\Sigma\partial_\mu\Sigma^\dagger) - \frac{B_0 f^2}{2}\,\mathrm{tr}(M\Sigma^\dagger + M^\dagger\Sigma)) \; -W'\left(\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)\right)^2$$

$$+ \;\frac{\ell_7 B_0^2}{16}\left[\mathrm{tr}(M\Sigma^\dagger - M^\dagger\Sigma)\right]^2 \; + \ldots$$

- ℓ_7 contributes $\Delta M_\pi^2 \propto (m_u - m_d)^2/m_s$, which is leading order in SU(3) ChPT, but NLO in standard SU(2) power counting
- To justify keeping the ℓ_7 term, we use the following nonstandard power counting [$m \sim m_u + m_d$, $\varepsilon \sim m_u - m_d$]

$$m \sim p^2 \sim a^2 > \epsilon^2 > ma \sim a^3 > a\epsilon^2 > m^2 \sim ma^2 \sim a^4 \ldots$$

- Formally justify by treating $\varepsilon \sim a^{(1+\delta)}$ with $0 < \delta < 0.5$

- Real justification is that ε^2 term gives the leading contribution to isospin breaking, and is not renormalized by loop contributions
- Nominally subleading terms (e.g. m^2 terms) may be numerically larger but do not lead to qualitatively new effects
- We have also considered the impact of the ma and a^3 terms

Including EM effects

- In continuum ChPT leading term from EM is:

$$\mathcal{V}_{\rm EM} = -\frac{f^2}{4} c_{\rm EM}\, \mathrm{tr}(\Sigma\tau_3\Sigma^\dagger\tau_3) \qquad c_{\rm EM} \propto \alpha_{\rm EM} \qquad c_{\rm EM} > 0$$

[Witten 83]

- We treat this as of LO: $\alpha_{EM} \sim a^2 \sim m$

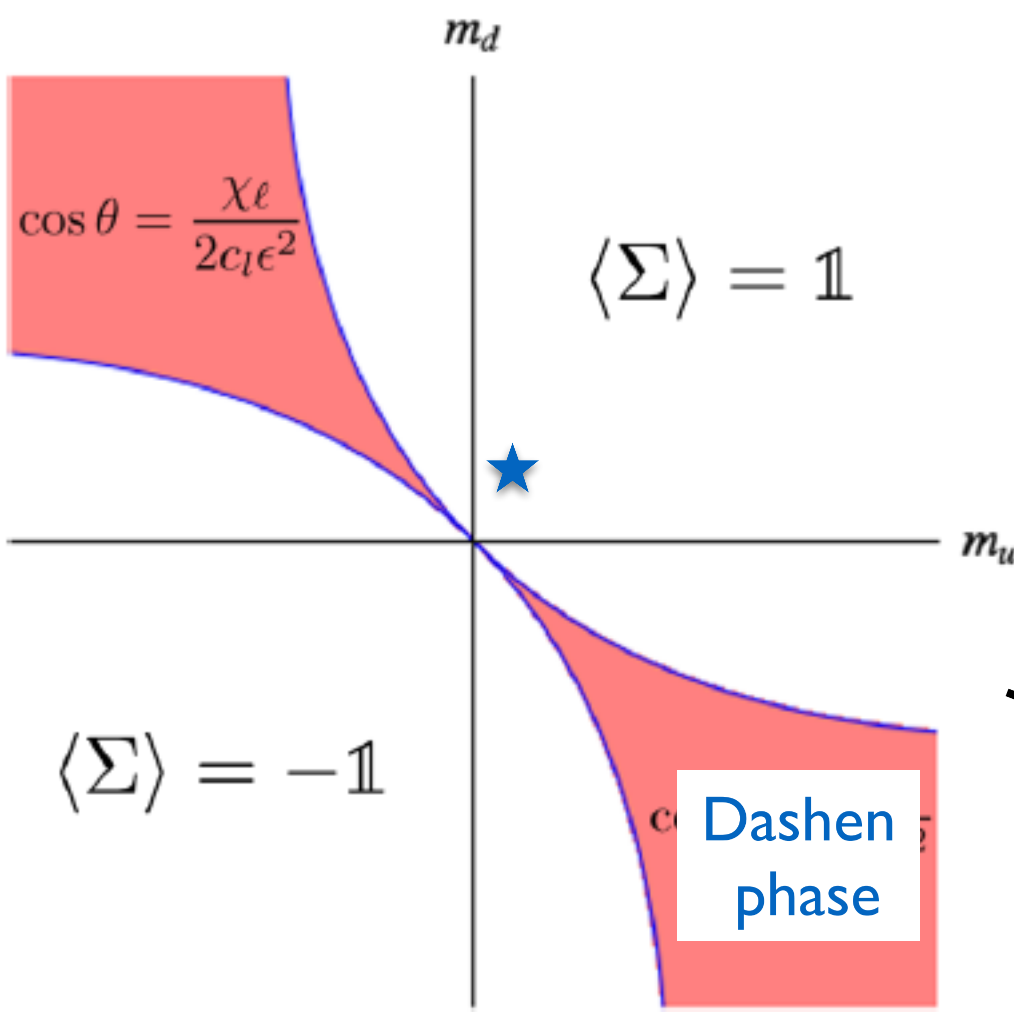
- Can be absorbed by shifting W' and ℓ_7 terms in a≠0 chiral Lagrangian

$$4\,\mathrm{tr}\left(\Sigma\tau_3\Sigma^\dagger\tau_3\right) = \left[\mathrm{tr}\left(\Sigma+\Sigma^\dagger\right)\right]^2 - \left[\mathrm{tr}\left([\Sigma-\Sigma^\dagger]\tau_3\right)\right]^2 - 8$$

- Phase diagram completely unchanged (shifts cancel)
- Only effect of c_{EM} term is to increase $m(\pi^+)^2$ by $2c_{EM}$ uniformly
- Dominant effect of EM with Wilson-like fermions is shift in bare quark masses proportional to α_{EM}/a, differing for up and down quarks

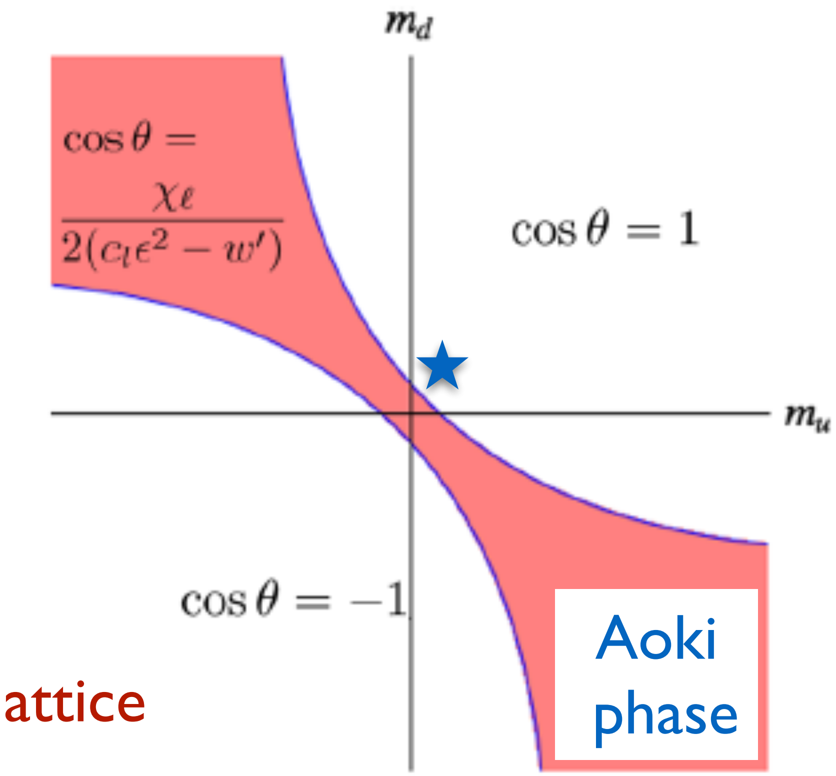
WχPT: SU(2) with $m_u \neq m_d$ & $\alpha_{EM} \neq 0$

NLO in continuum



Aoki scenario

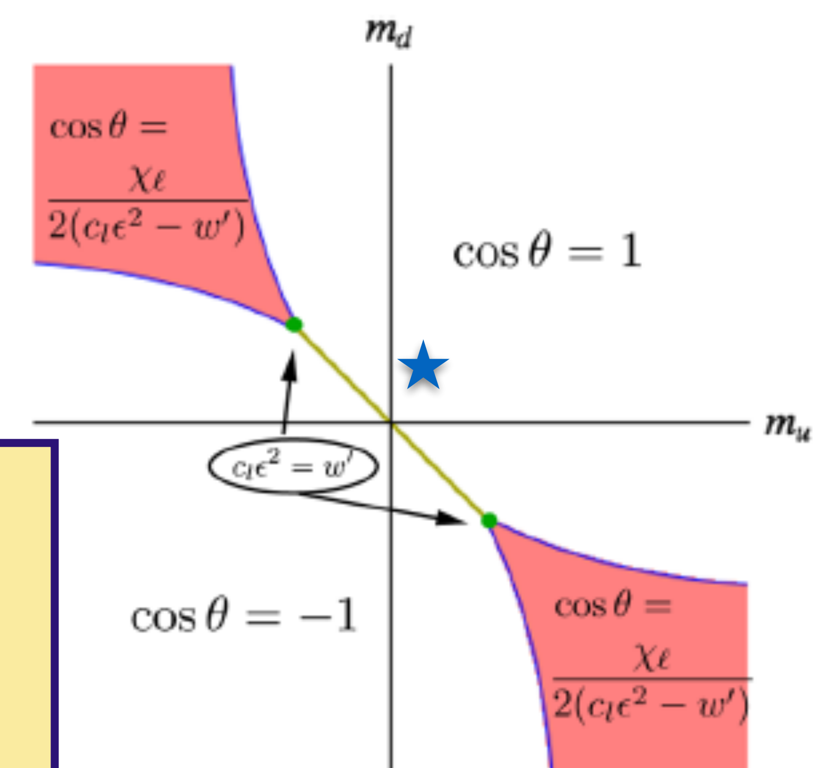
$w' < 0$



NLO on lattice

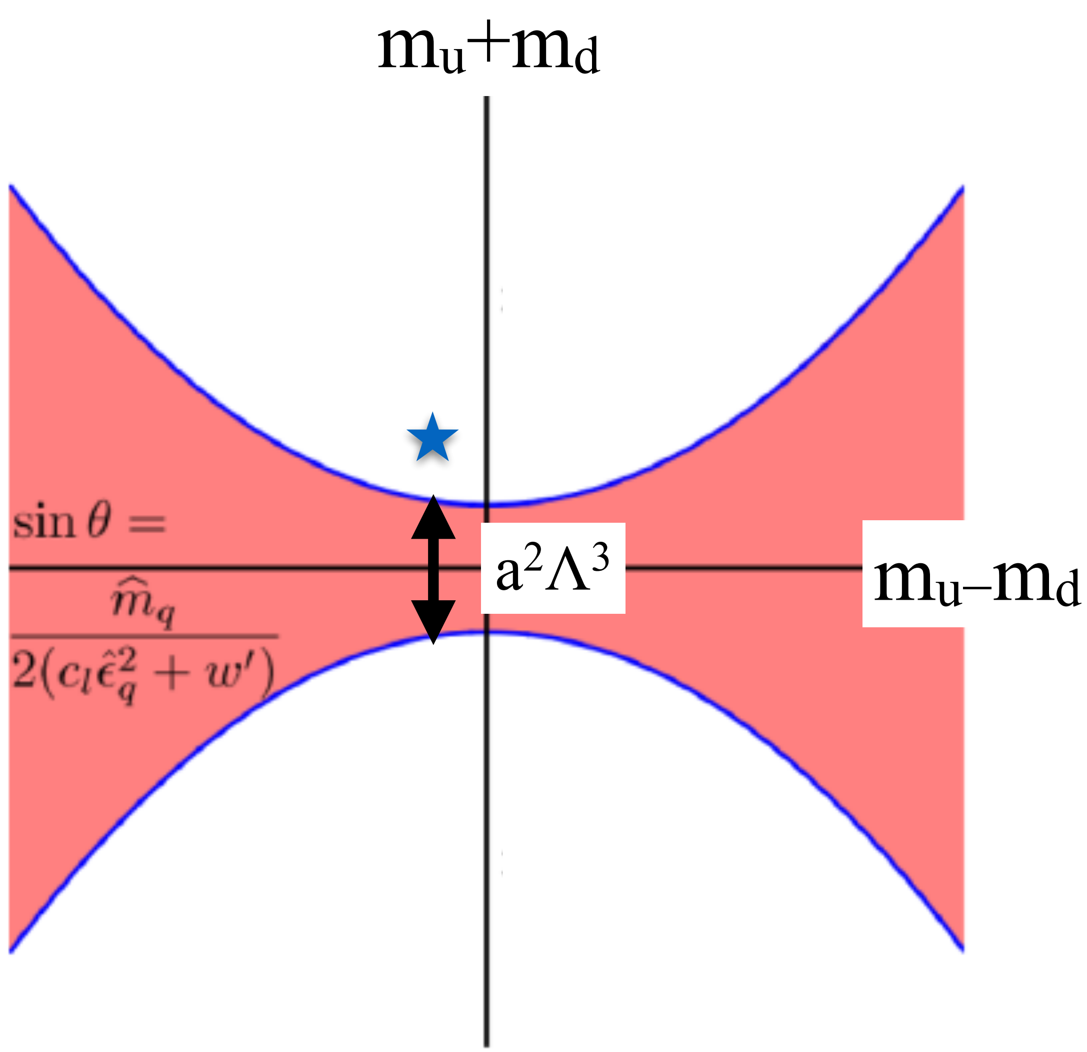
$w' > 0$

1st-order scenario

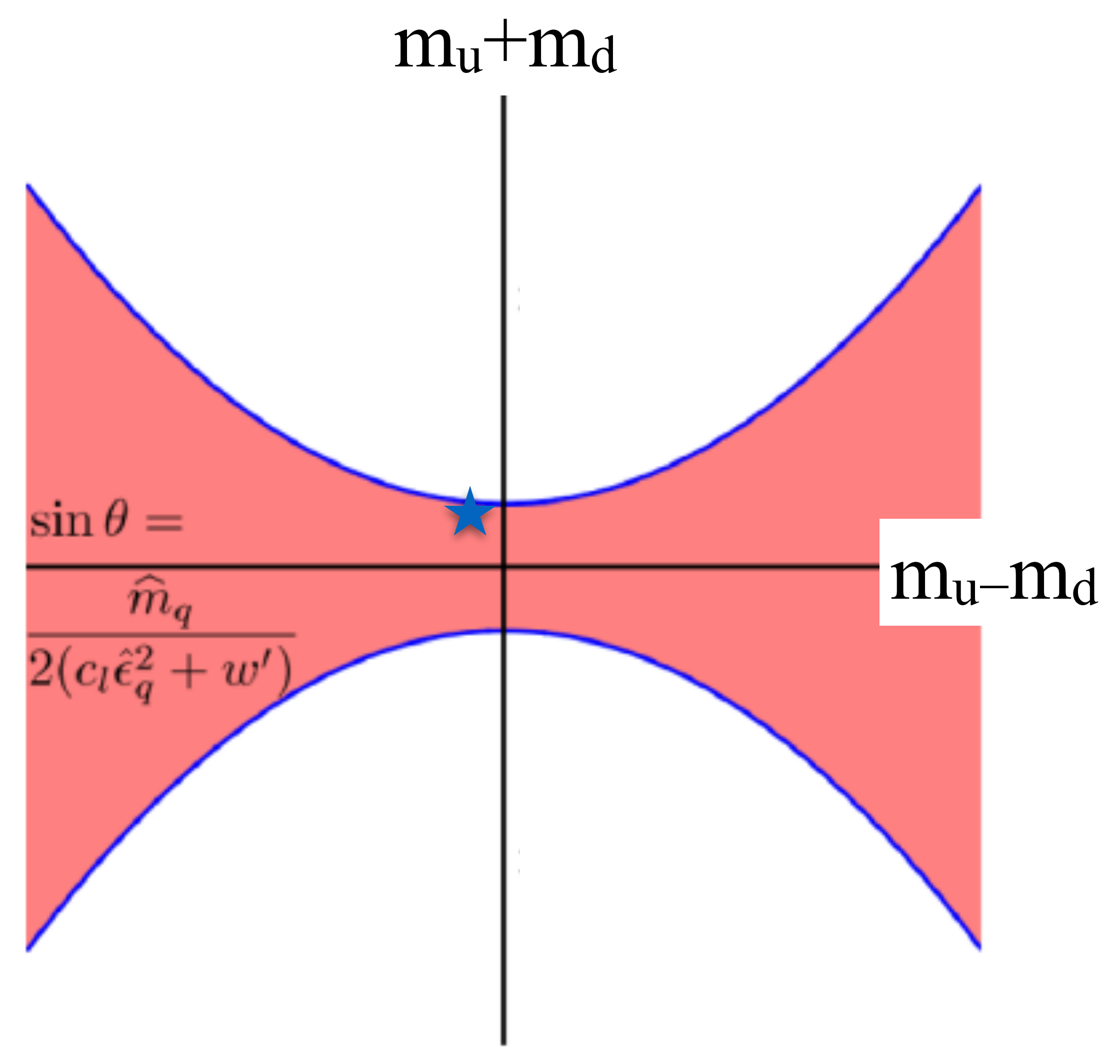


- Aoki phase = Dashen phase
- Nondegeneracy increases size of Aoki phase
- EM does not affect phase diagram

Issue for simulations



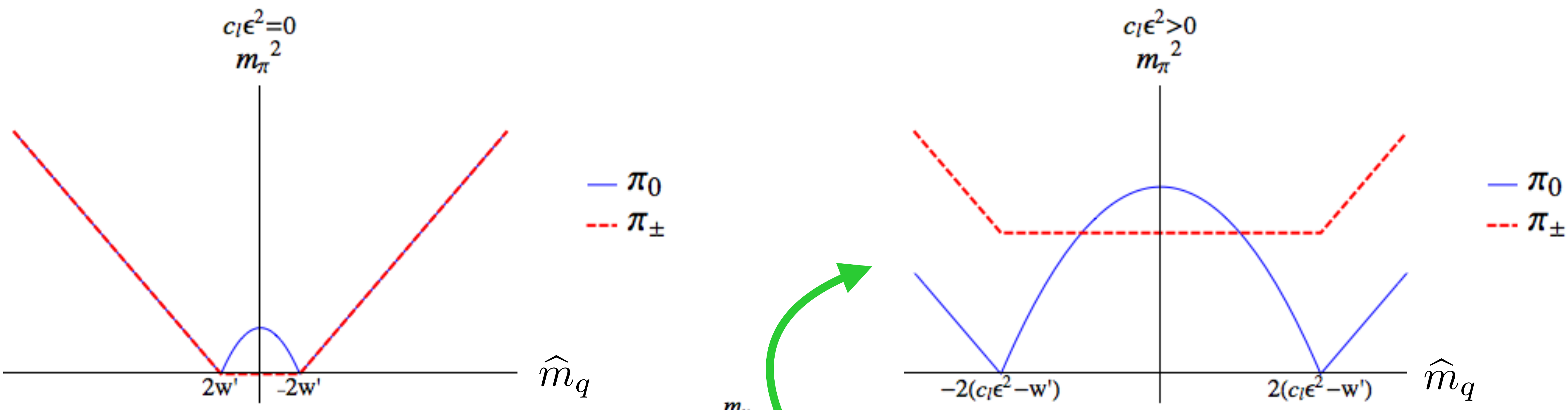
or

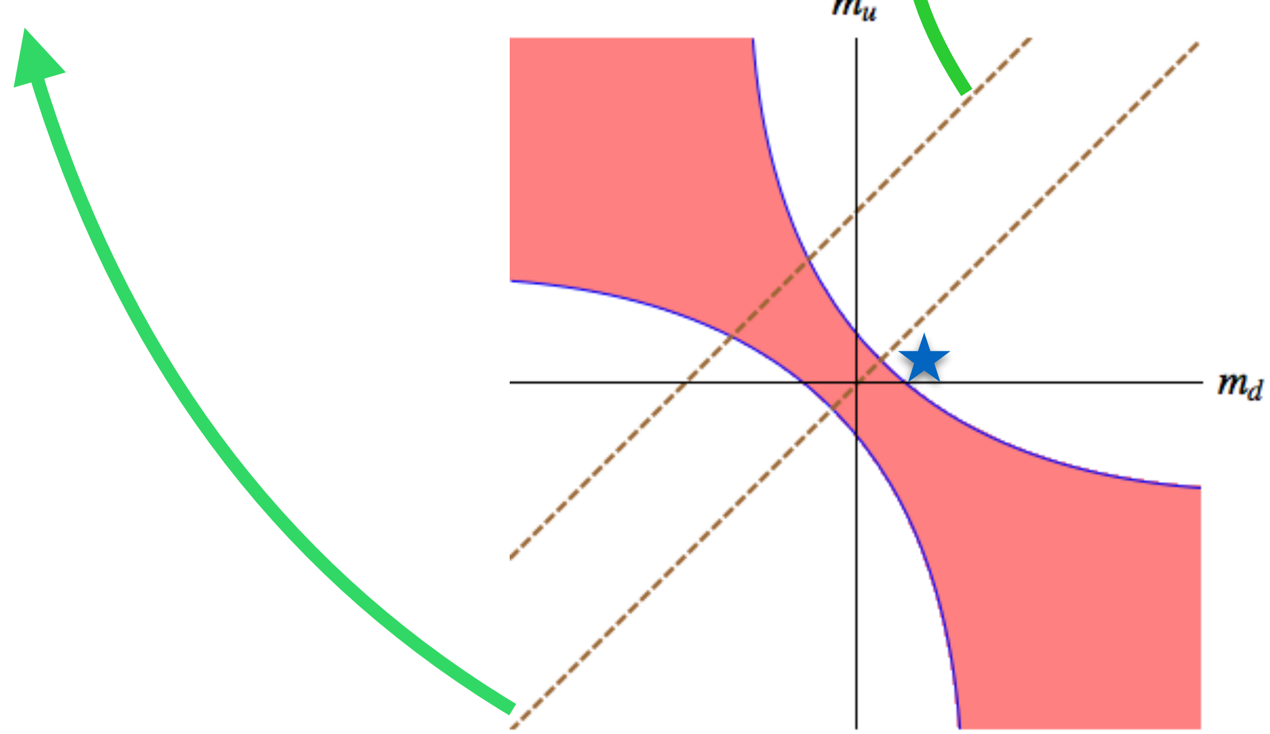


?

In fact, present simulations appear to be outside the unphysical phase

Pion masses

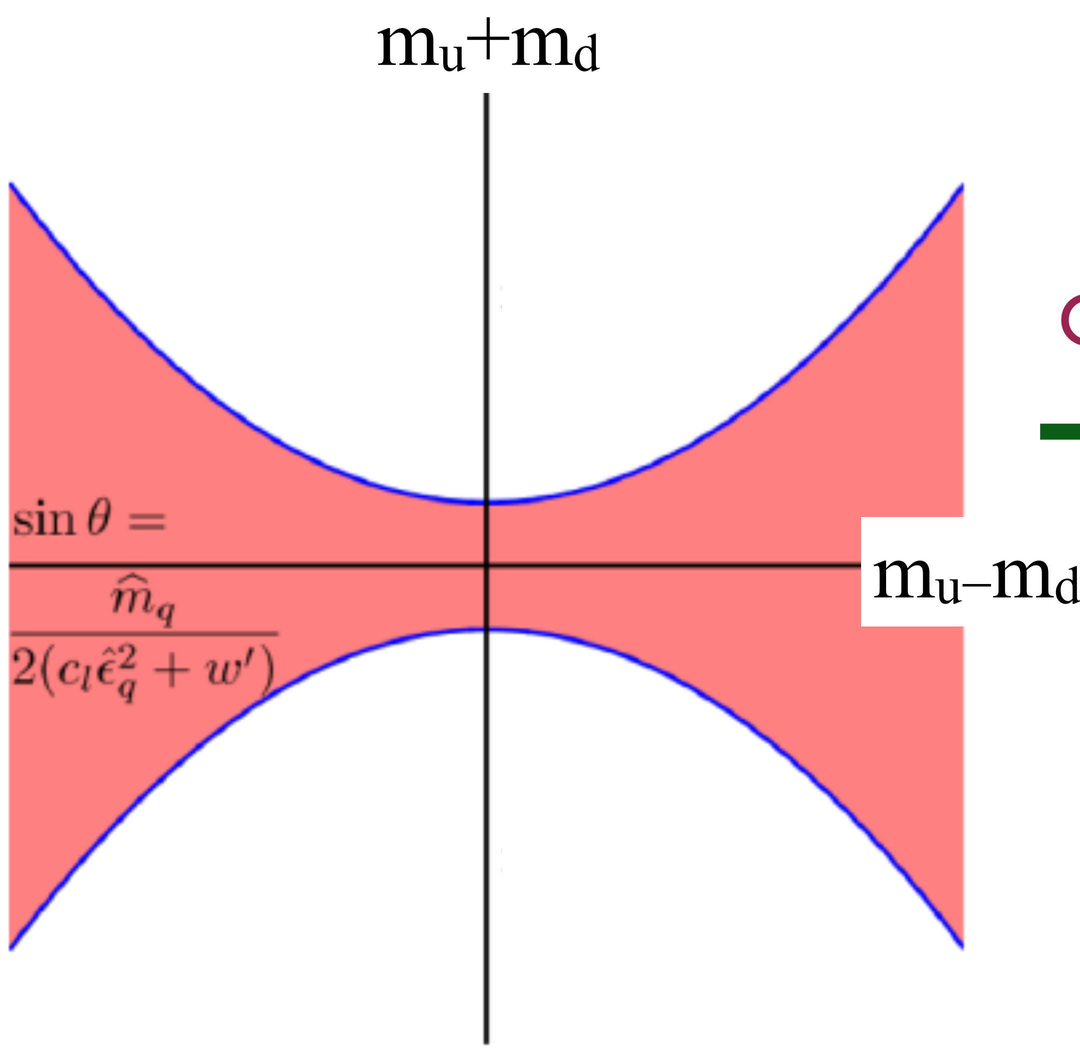




charged pion masses
further shifted
upwards by EM
(uniformly across phase plane)

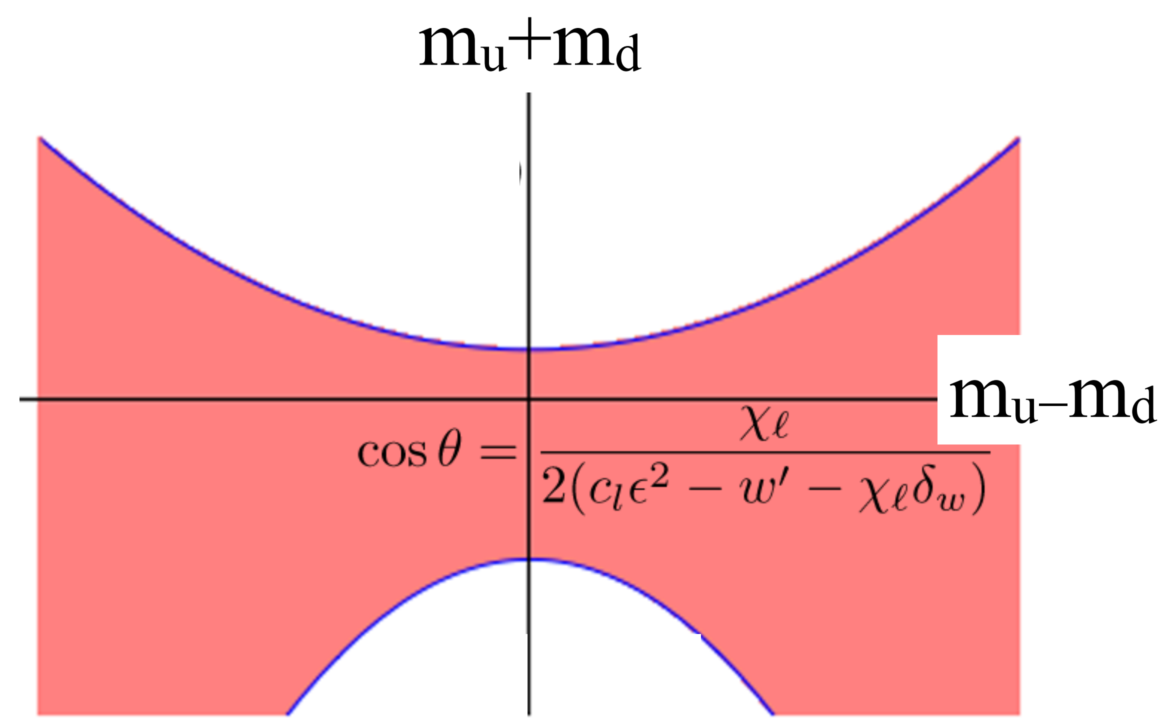
Impact of higher order terms

$$\mathcal{V}_{A^3} = \underbrace{-W\,\mathrm{tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\,\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)}_{O(am)} - \underbrace{\frac{W_{3,3}}{f^2}\,\mathrm{tr}((A^\dagger\Sigma)^3 + (\Sigma^\dagger A)^3)}_{O(a^3)}$$



Aoki scenario

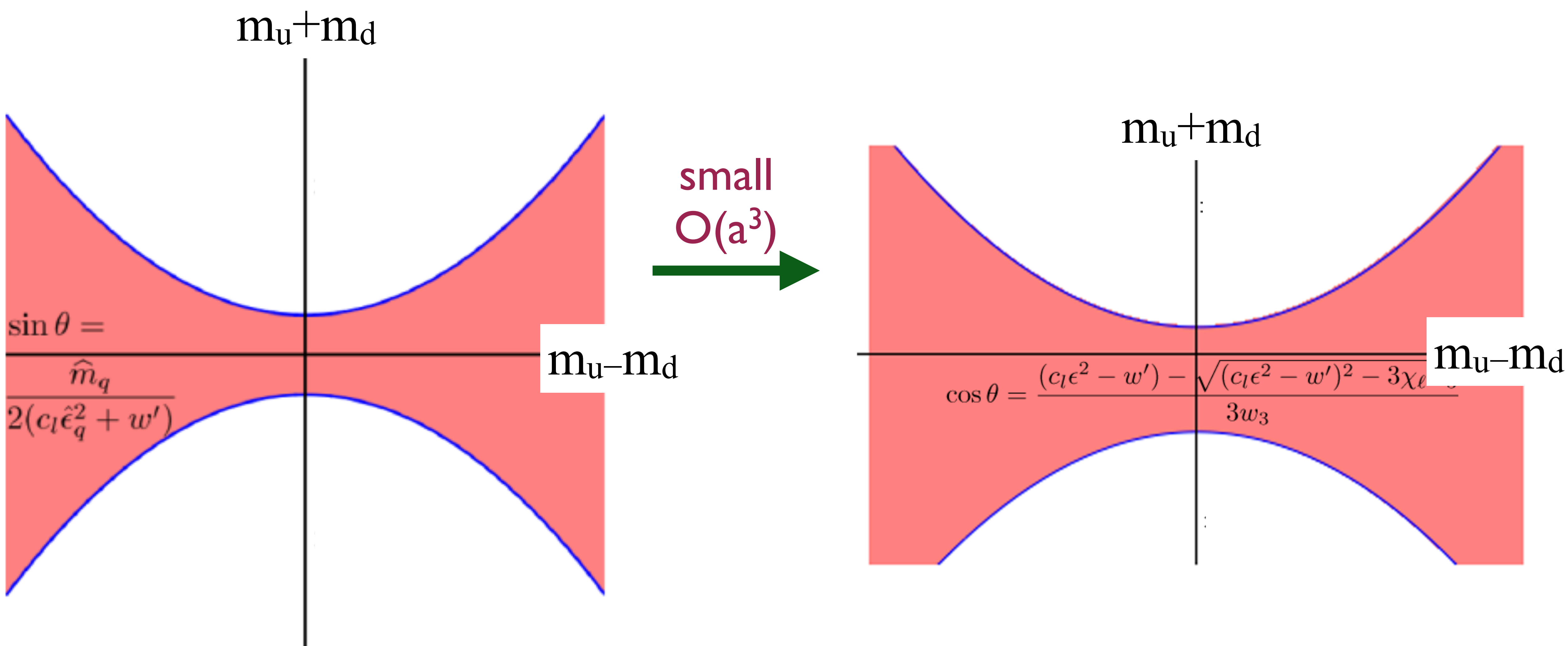
O(am)



up-down asymmetry

Impact of higher order terms

$$\mathcal{V}_{A^3} = \underbrace{-W\,\mathrm{tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\,\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)}_{\text{O(am)}} - \underbrace{\frac{W_{3,3}}{f^2}\,\mathrm{tr}((A^\dagger\Sigma)^3 + (\Sigma^\dagger A)^3)}_{\text{O(a}^3\text{)}}$$

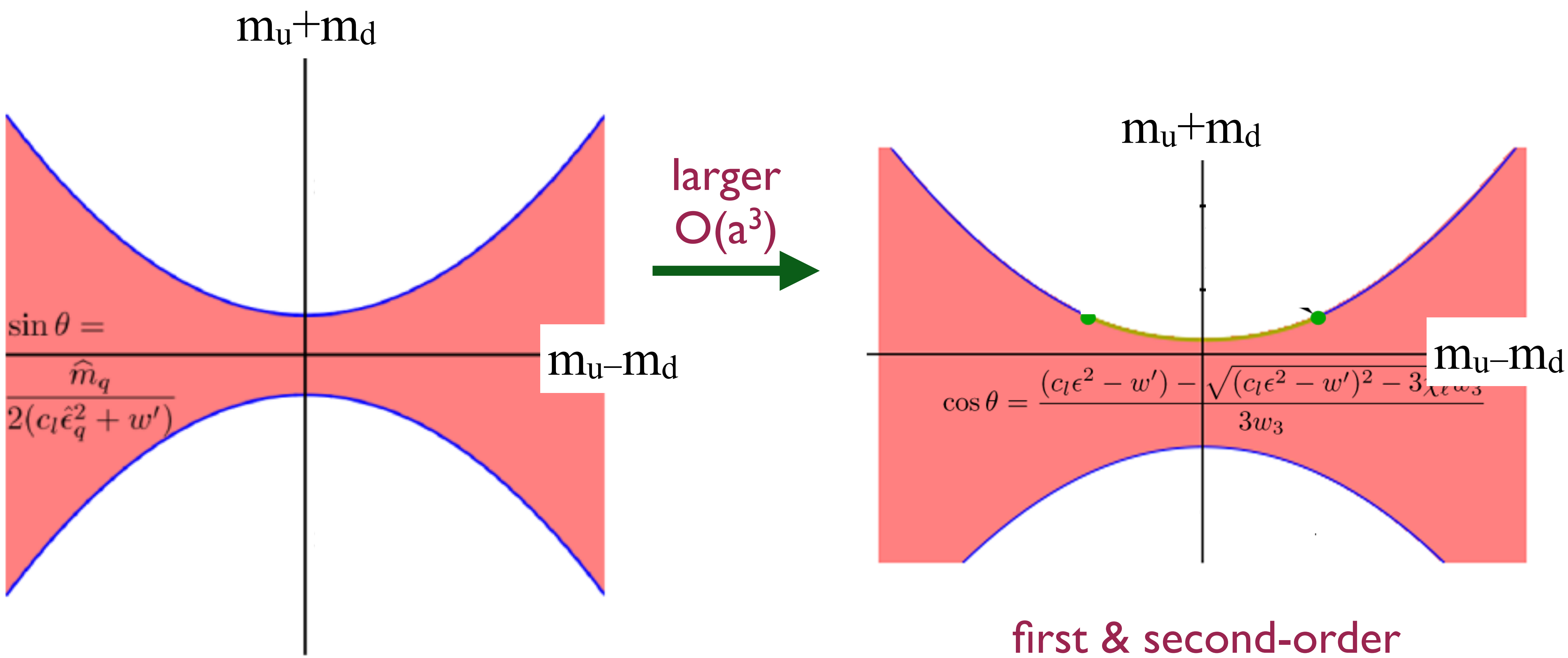


Aoki scenario

vertical shift

Impact of higher order terms

$$\mathcal{V}_{A^3} = \underbrace{-W\,\mathrm{tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\,\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)}_{\text{O(am)}} - \underbrace{\frac{W_{3,3}}{f^2}\,\mathrm{tr}((A^\dagger\Sigma)^3 + (\Sigma^\dagger A)^3)}_{\text{O(a}^3\text{)}}$$



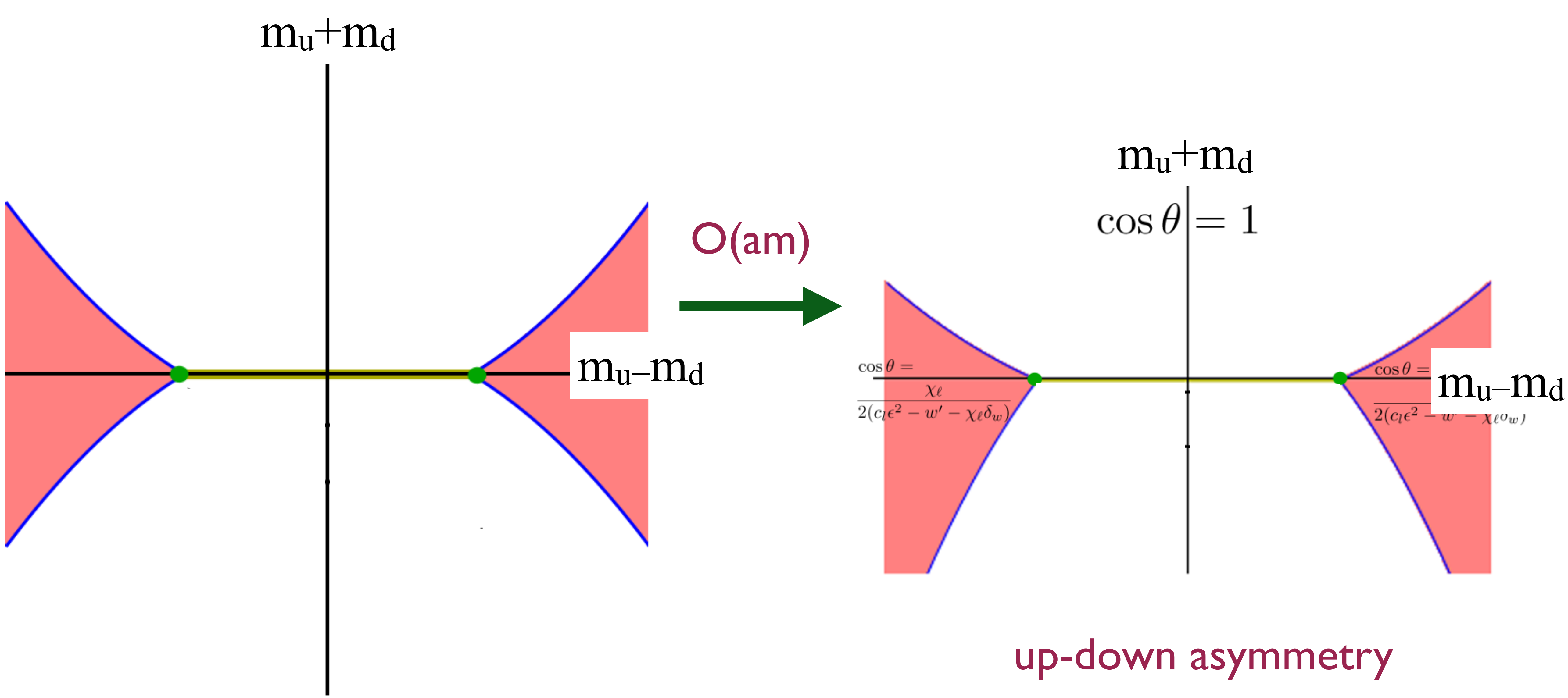
Aoki scenario

first & second-order combined

Impact of higher order terms

$$\mathcal{V}_{A^3} = -W\,\mathrm{tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\,\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A) - \frac{W_{3,3}}{f^2}\,\mathrm{tr}((A^\dagger\Sigma)^3 + (\Sigma^\dagger A)^3)$$

O(am) O(a^3)

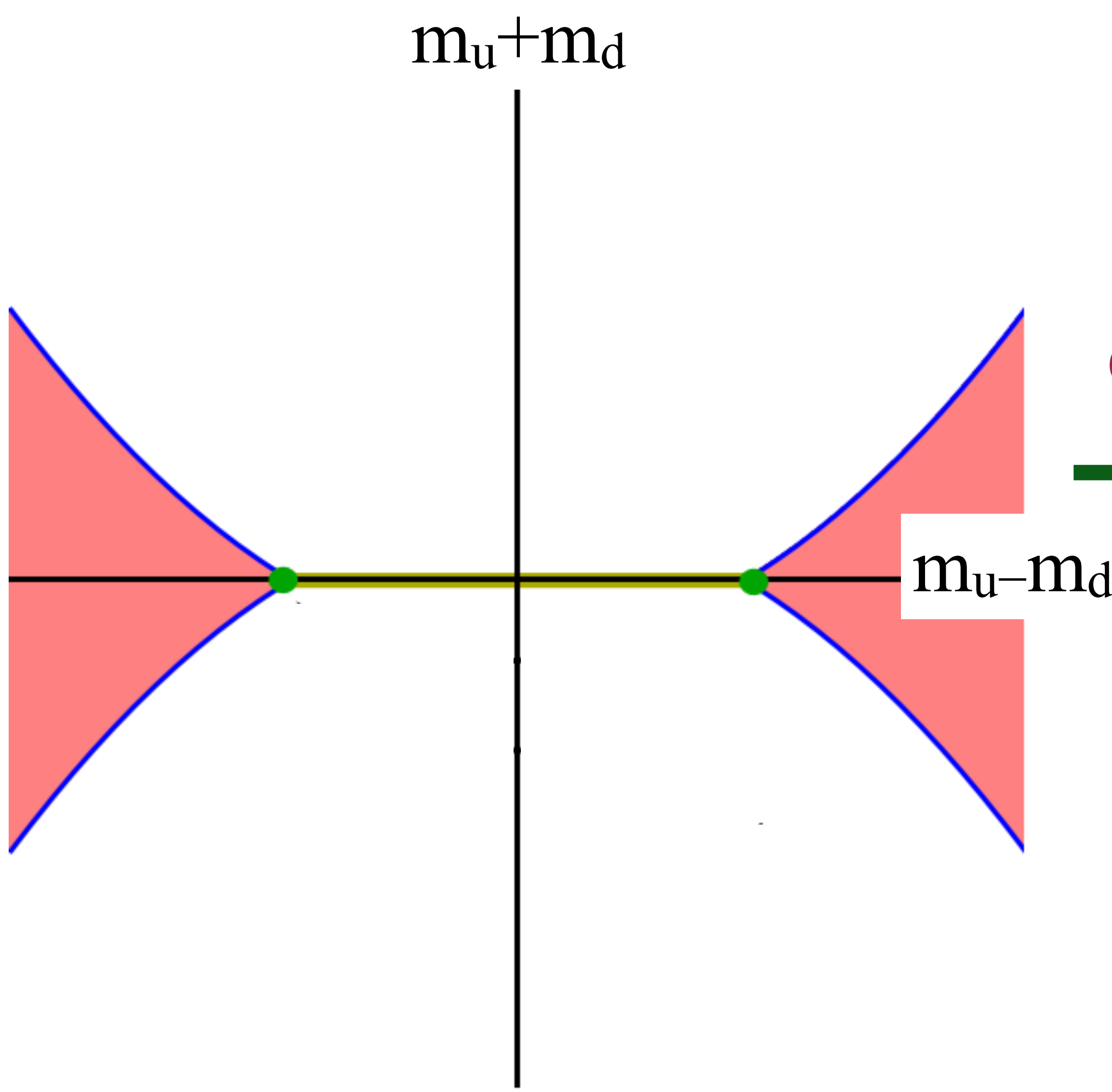


First-order scenario

up-down asymmetry

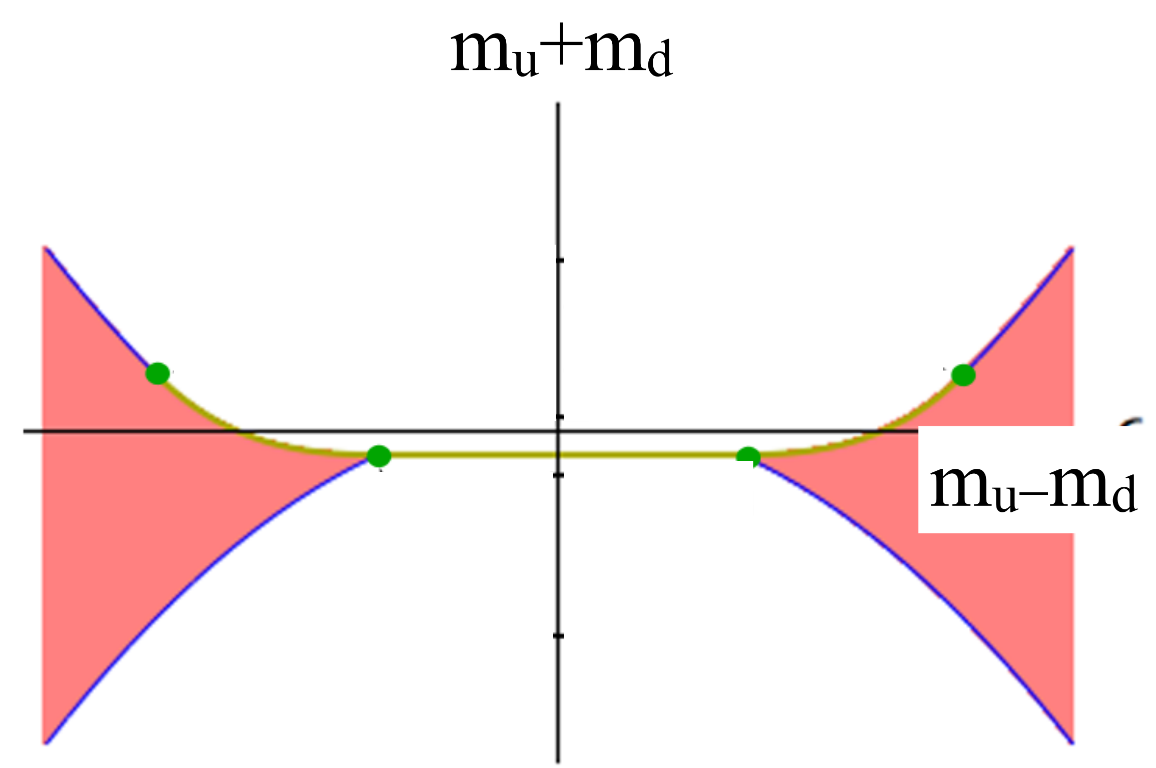
Impact of higher order terms

$$\mathcal{V}_{A^3} = \underbrace{-W\,\mathrm{tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\,\mathrm{tr}(A^\dagger\Sigma + \Sigma^\dagger A)}_{O(am)} - \underbrace{\frac{W_{3,3}}{f^2}\,\mathrm{tr}((A^\dagger\Sigma)^3 + (\Sigma^\dagger A)^3)}_{O(a^3)}$$



First-order scenario

O(a^3)



first & second-order plus shift

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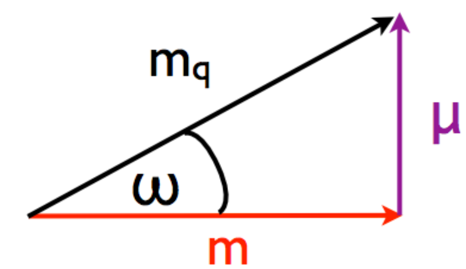
Twisted-mass lattice QCD

- "Twisting" ⇒ flavor nonsinglet axial rotation to common u-d mass

$$m_q \to m_q e^{i\gamma_5 \tau_i \omega}$$



- In the continuum, ω is redundant—changing it has no physical effect
- On the lattice, results do depend on ω, because axial symmetries are broken by the Wilson term [Frezzotti, Grassi, Sint & Weisz 01]
- Twisting is used mainly because of automatic O(a) improvement at maximal twist (ω=π/2) [Frezzotti & Rossi 04]
- Achieving maximal twist requires tuning m→0 i.e. $\kappa \to \kappa_c$
  - Nontrivial because of additive mass renormalization $\Delta m \sim \alpha_s/a$
- Standard tuning condition is to set $m_{PCAC}=0$

$$\langle \pi^+ | \overline{u} \gamma_\mu \gamma_5 d | 0 \rangle \Big|_{m=m_c} = 0$$

Twisting in the presence of isospin breaking

- Standard choice without EM is to twist in a perpendicular direction in isospin space to the nondegeneracy—quark determinant remains real

$$\overline{\psi}(\not{D} + m_q e^{i\gamma_5\tau_1\omega} + \epsilon_q\tau_3)\psi = \overline{\psi}(\not{D} + m\mathbb{1} + i\mu\gamma_5\tau_1 + \epsilon_q\tau_3)\psi$$

[Frezzotti & Rossi 04, Used by ETMC for strange & charm]

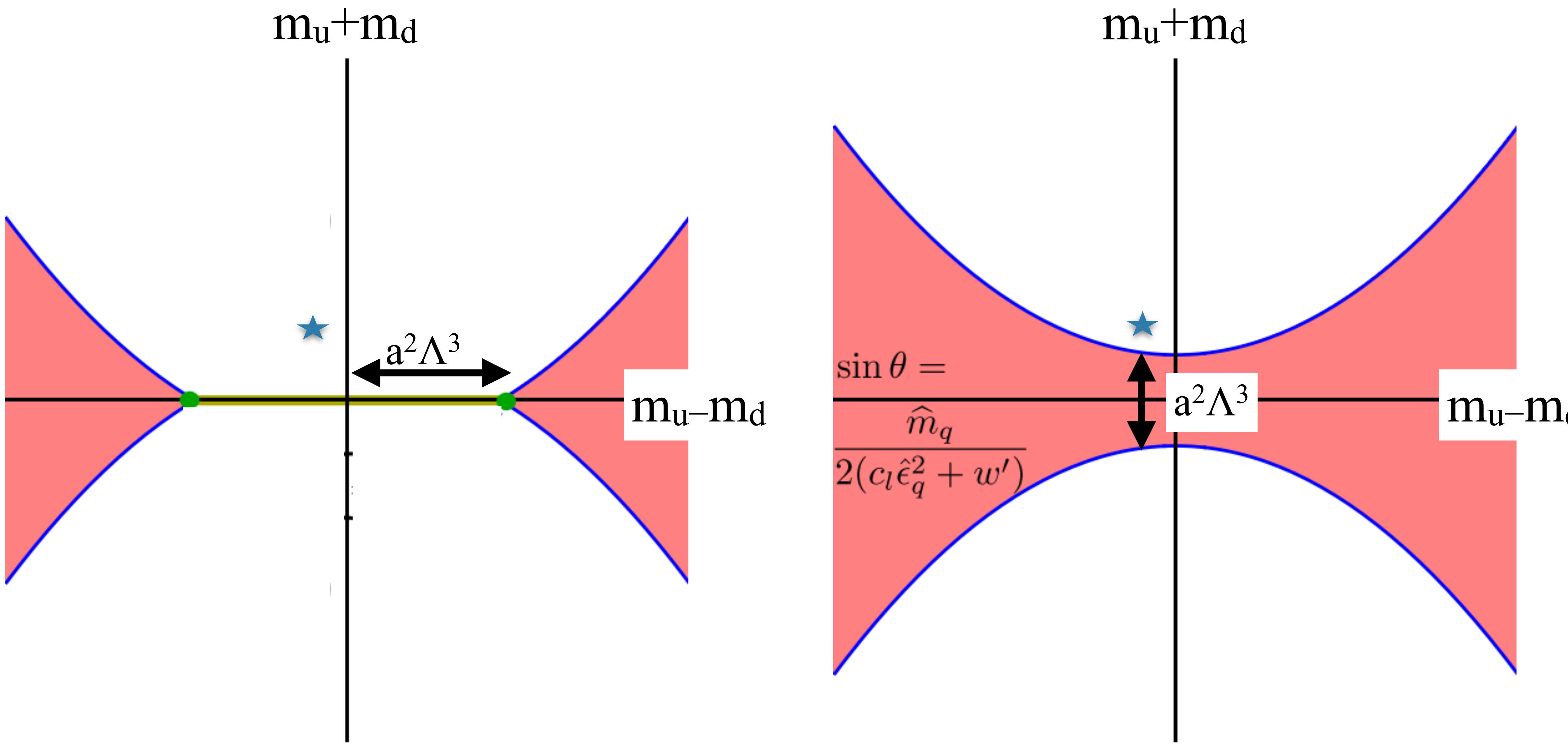
- Cannot use with EM since photon couples to a mix of vector and axial currents, and the latter are not conserved with Wilson-like fermions

- In a lattice theory one **must twist in same direction as nondegeneracy**, implying complex determinant

- RM123 collab. use such a twist, but avoid the complex determinant by doing a first-order perturbative expansion in $m_u - m_d$ & α_{EM}

- Using tmChPT we study the theory without need for such an expansion

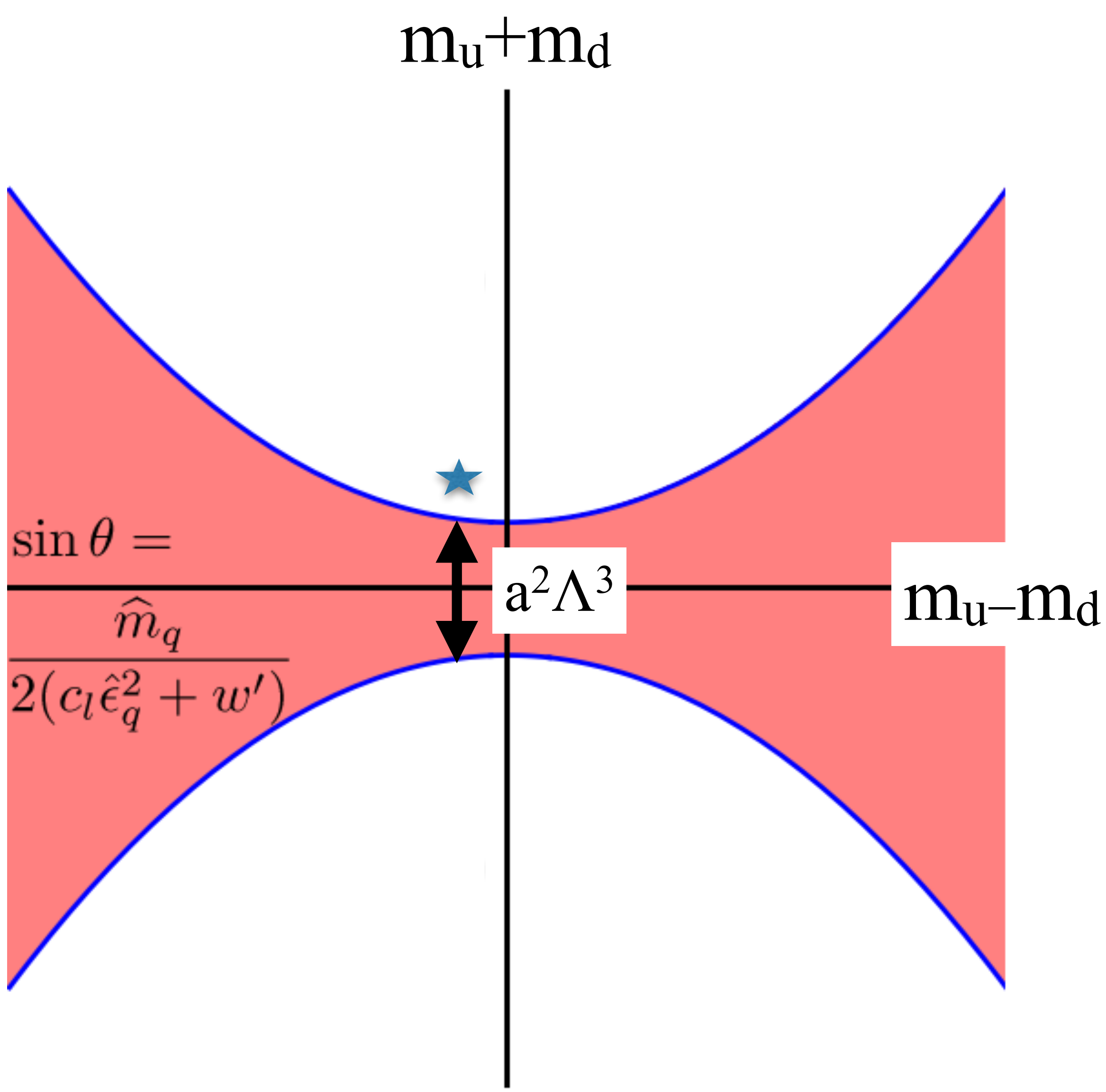
tmχPT at max. twist: $m_u \neq m_d$ & $\alpha_{EM} \neq 0$



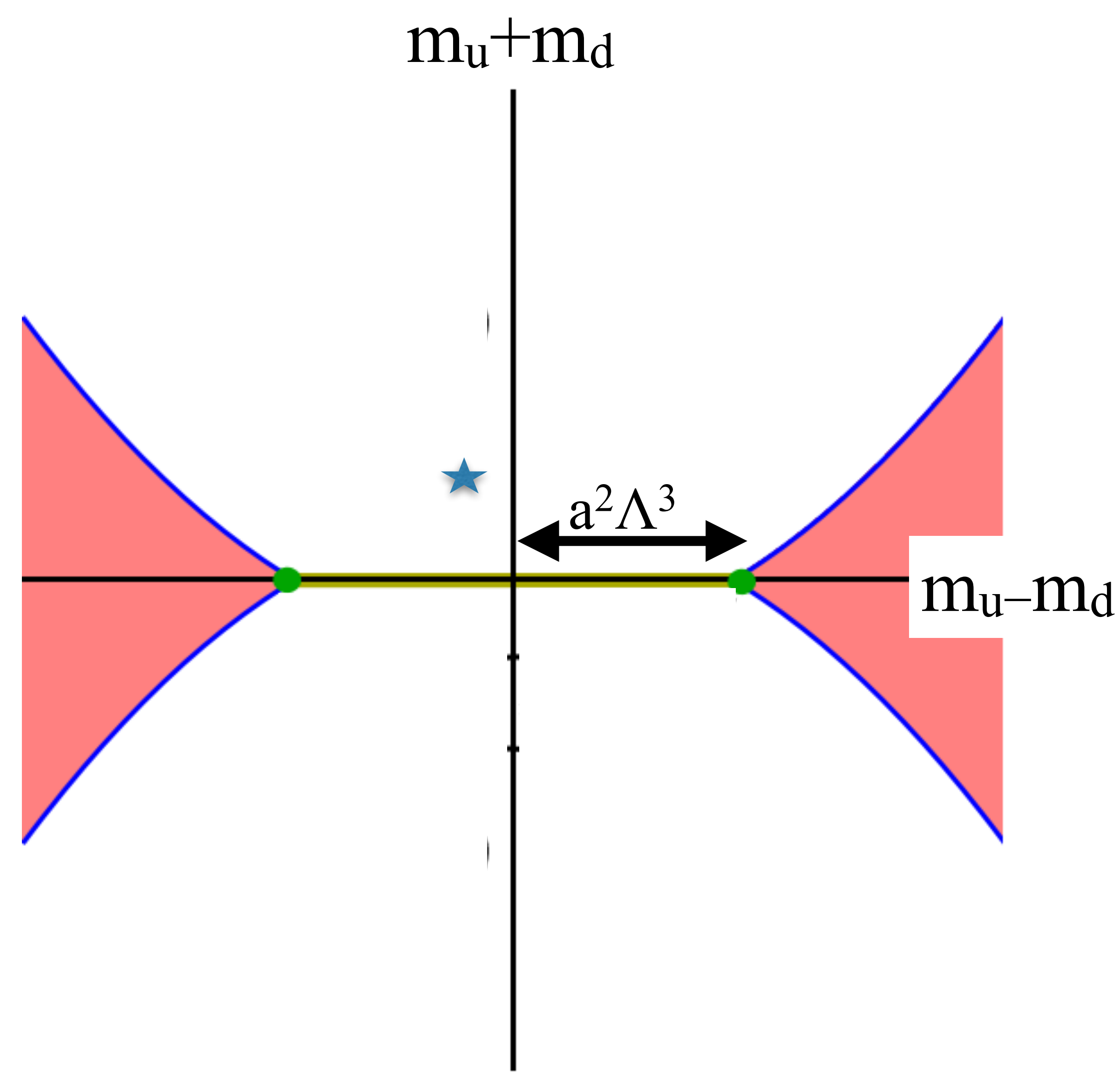
Aoki Scenario (**w'<0**)   First-Order Scenario (**w'>0**)

- Roles of two scenarios interchanged
- Again, simulations appear to lie outside unphysical phase

WχPT at max. twist: $m_u \neq m_d$ & $\alpha_{EM} \neq 0$



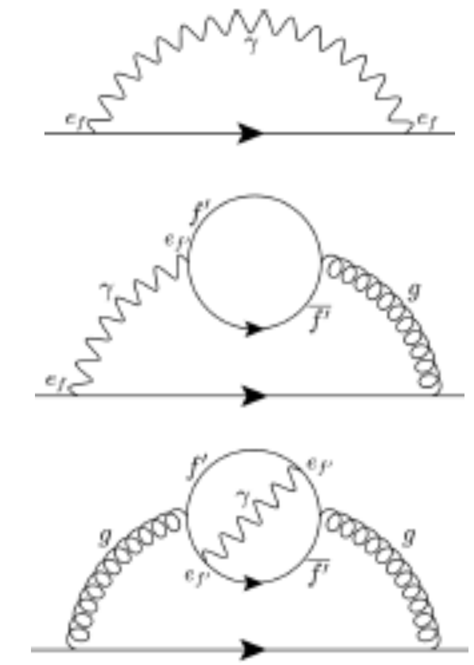
Aoki Scenario (w'<0)



First-Order Scenario (w'>0)

- Roles of two scenarios interchanged
- Again, simulations appear to lie outside unphysical phase

Tuning to max twist with $\alpha_{EM} \neq 0$



- Up & down critical masses differ by $O(\alpha_{EM}/a)$
- "$m_{PCAC}=0$" method of tuning fails
- RM123 collab. use PQ variant of $m_{PCAC}=0$
- Untuned theory has $\theta_{QCD} \neq 0$
- To study tuning, need PQtmχPT for $m_u \neq m_d$ & $\theta_{QCD} \neq 0$!
  - We find that PQ $m_{PCAC}=0$ method fails (only tune one linear combination)
  - We propose an alternative method—minimize the pion masses (for the distant future when such simulations are possible!)
  - RM123 avoid our criticism since they expand perturbatively about the isospin-symmetric theory and use the electroquenched approximation

Conclusions

- ChPT allows one to study the low-energy structure of lattice QCD in the presence of isospin breaking
- The Aoki phase turns out to be part of the CP-violating Dashen/Creutz phase
- Nondegeneracy makes this phase slightly wider, and thus slightly more dangerous for simulations
  - In practice, has not so far been a problem
- Tuning to maximal twist in the presence of EM in an unquenched, non-perturbative theory is challenging

Thank you!
Questions?

Backup slides

Tuning to Maximal Twist with EM

- The twisted quark mass matrix is

$$m\mathbb{1} + \epsilon\tau_3 + i\mu\gamma_5\tau_3 + i\eta\gamma_5 = \begin{pmatrix} m_u + i\mu_u\gamma_5 & 0 \\ 0 & m_d - i\mu_d\gamma_5 \end{pmatrix}$$

- One tuning proposal is to introduce a pair of valence quarks (u_V, d_V) that have the same untwisted masses & charges as the corresponding sea quark (u_S, d_S) but opposite twisted masses [RM123 Collab. 2013]

$$\Psi^\top = (u_S, u_V, d_V, d_S)$$

- The EM shift in the untwisted mass will be the same within each pair, so each of the (V,S) mass matrices will have the standard twisted form

$$\begin{pmatrix} m_u e^{i\omega_u\gamma_5\tau_3} & 0 \\ 0 & m_d e^{i\omega_d\gamma_5\tau_3} \end{pmatrix}$$

- Impose separate PCAC-like conditions for u & d quarks

$$\langle \pi^u_{SV} | \overline{u}_S \gamma_\mu \gamma_5 u_V | 0 \rangle \Big|_{m_u = m_{c,u}} = 0 \qquad \langle \pi^d_{SV} | \overline{d}_S \gamma_\mu \gamma_5 d_V | 0 \rangle \Big|_{m_d = m_{c,d}} = 0$$

Tuning to Maximal Twist with EM

- We have checked whether this condition is valid, using PQChPT (with $m_u \neq m_d$ and EM and $\theta_{QCD} \neq 0$)

- Need two ghosts and thus have graded $SU(4|2)_L \times SU(4|2)_R$ group
- We show that condensate in quark sector is constrained by symmetries

$$\langle \Sigma_{PQ} \rangle = \mathrm{diag}(e^{i\theta}, e^{-i\theta}, e^{i\theta}, e^{-i\theta})$$

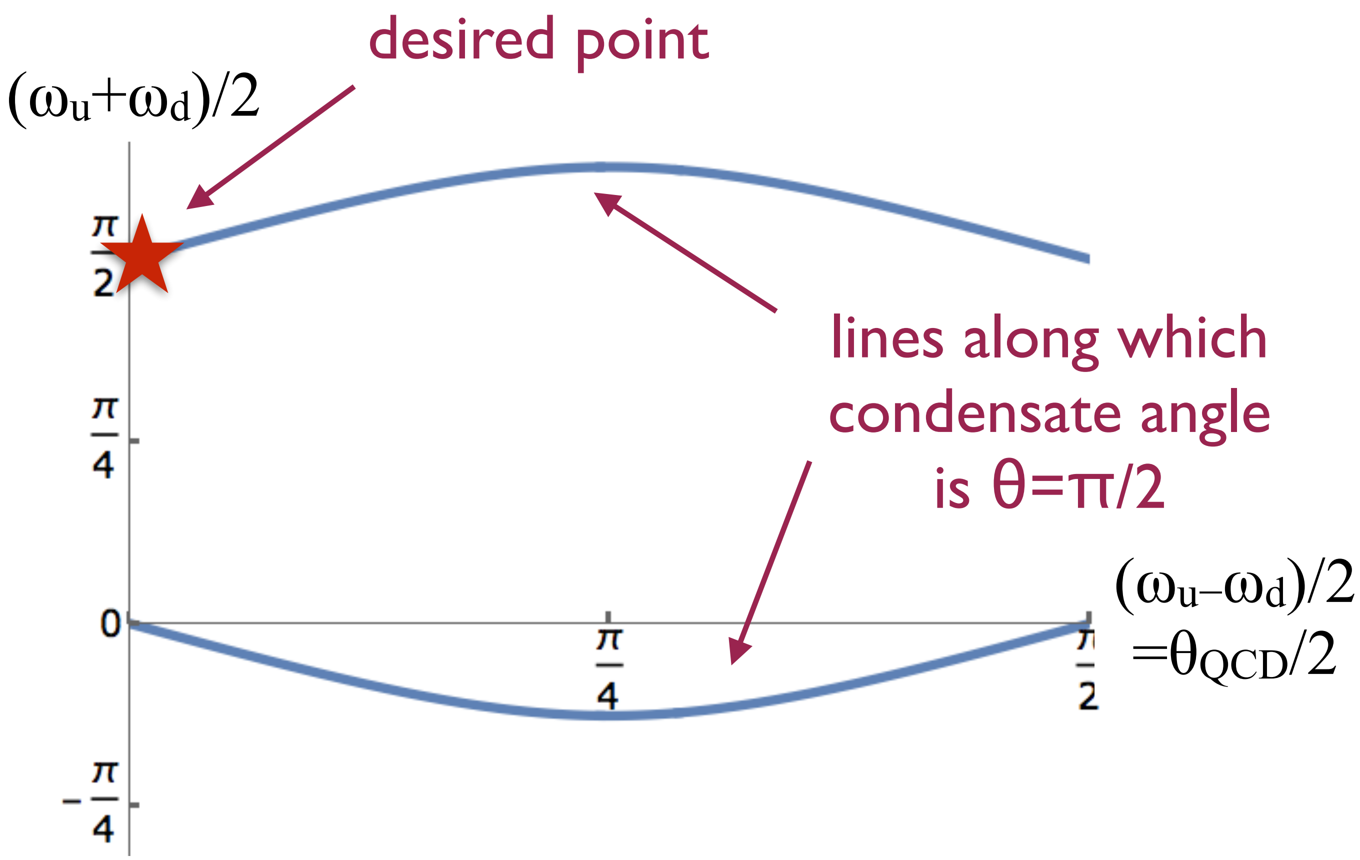
- Constructing the PQ axial currents at LO in ChPT one then finds that the PCAC conditions are not independent

$$\langle \pi^u_{SV} | \overline{u}_S \gamma_\mu \gamma_5 u_V | 0 \rangle \propto \cos\theta \qquad \langle \pi^d_{SV} | \overline{d}_S \gamma_\mu \gamma_5 d_V | 0 \rangle \propto \cos\theta$$

- Either condition alone (RHS=0) yields $\theta = \pi/2$

- ω_u & ω_d are only constrained by the tuning condition to lie along a line passing through the desired point $\omega_u = \omega_d = \pi/2$

Tuning to Maximal Twist with EM



- Within ChPT, the only condition we have found that picks out the desired point is to minimize the pion masses

- Using this condition in practice would be difficult since θ_{QCD} is nonzero

Nondegeneracy with orthogonal twists

- Twisting in an orthogonal direction to the nondegeneracy leads to a real fermion determinant [Frezzotti 04]

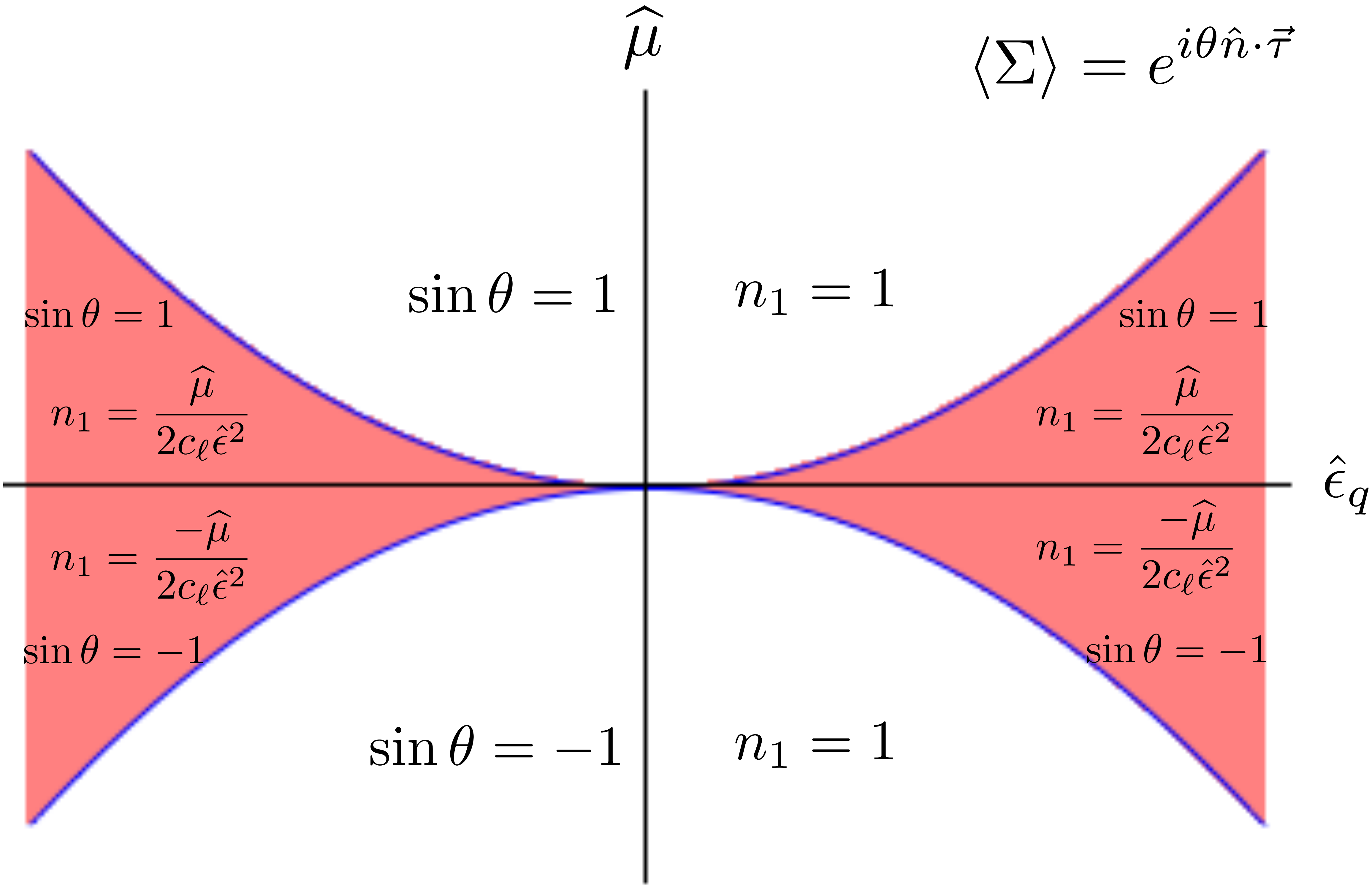
$$\overline{\psi}(\not{D} + m_q e^{i\gamma_5\tau_1\omega} + \epsilon_q\tau_3)\psi = \overline{\psi}(\not{D} + m\mathbb{1} + i\mu\gamma_5\tau_1 + \epsilon_q\tau_3)\psi$$

- Corresponding mass term in ChPT

$$B_0 M = \widehat{m}\mathbb{1} + i\widehat{\mu}\tau_1 + \hat{\epsilon}_q\tau_3$$

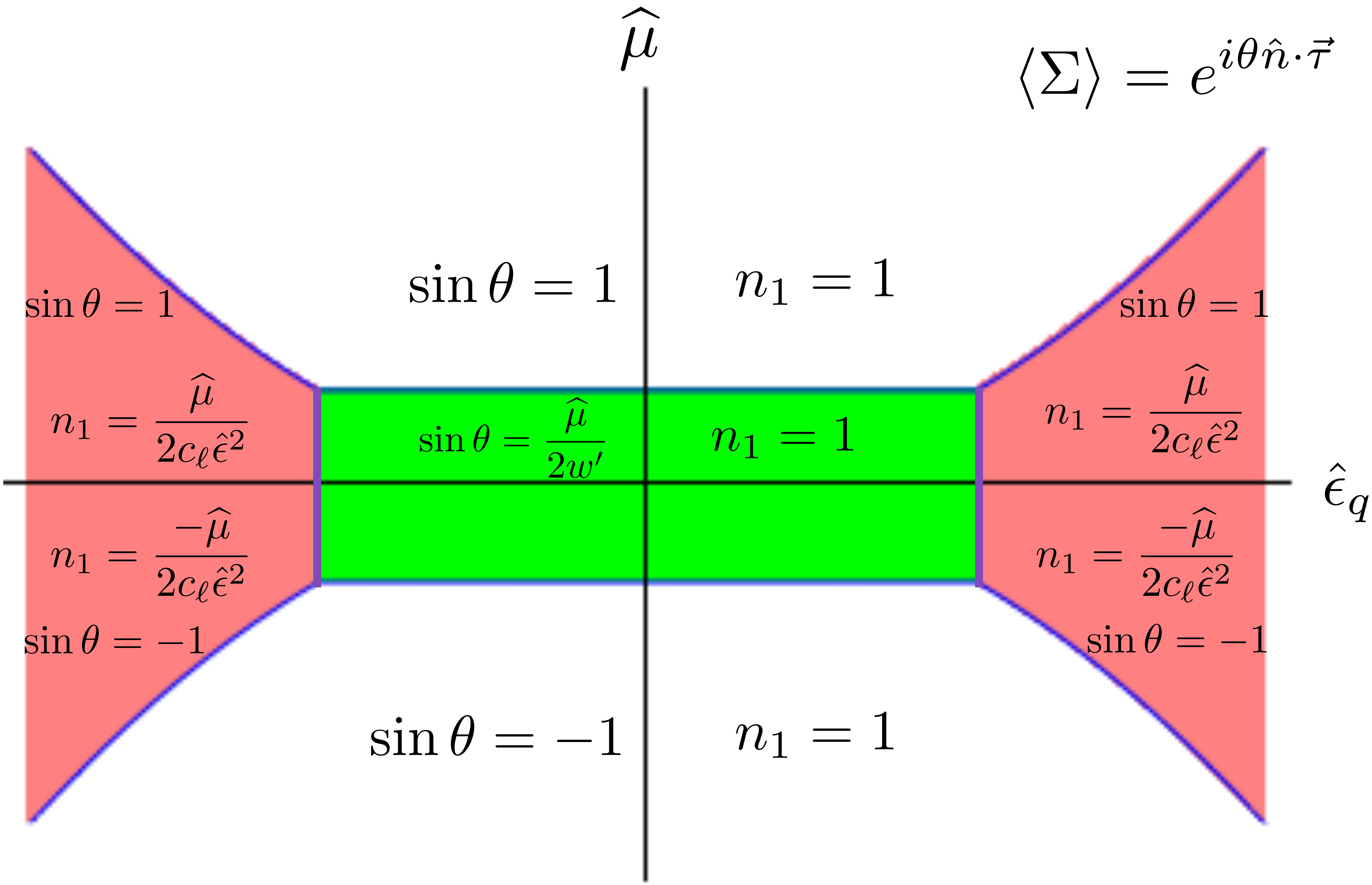
- As the twisted mass, μ, does not mix with any other operators in the Lagrangian, it is only renormalized multiplicatively

Phase Diagram at maximal twist



Aoki Scenario and the continuum ($w' \leq 0$)

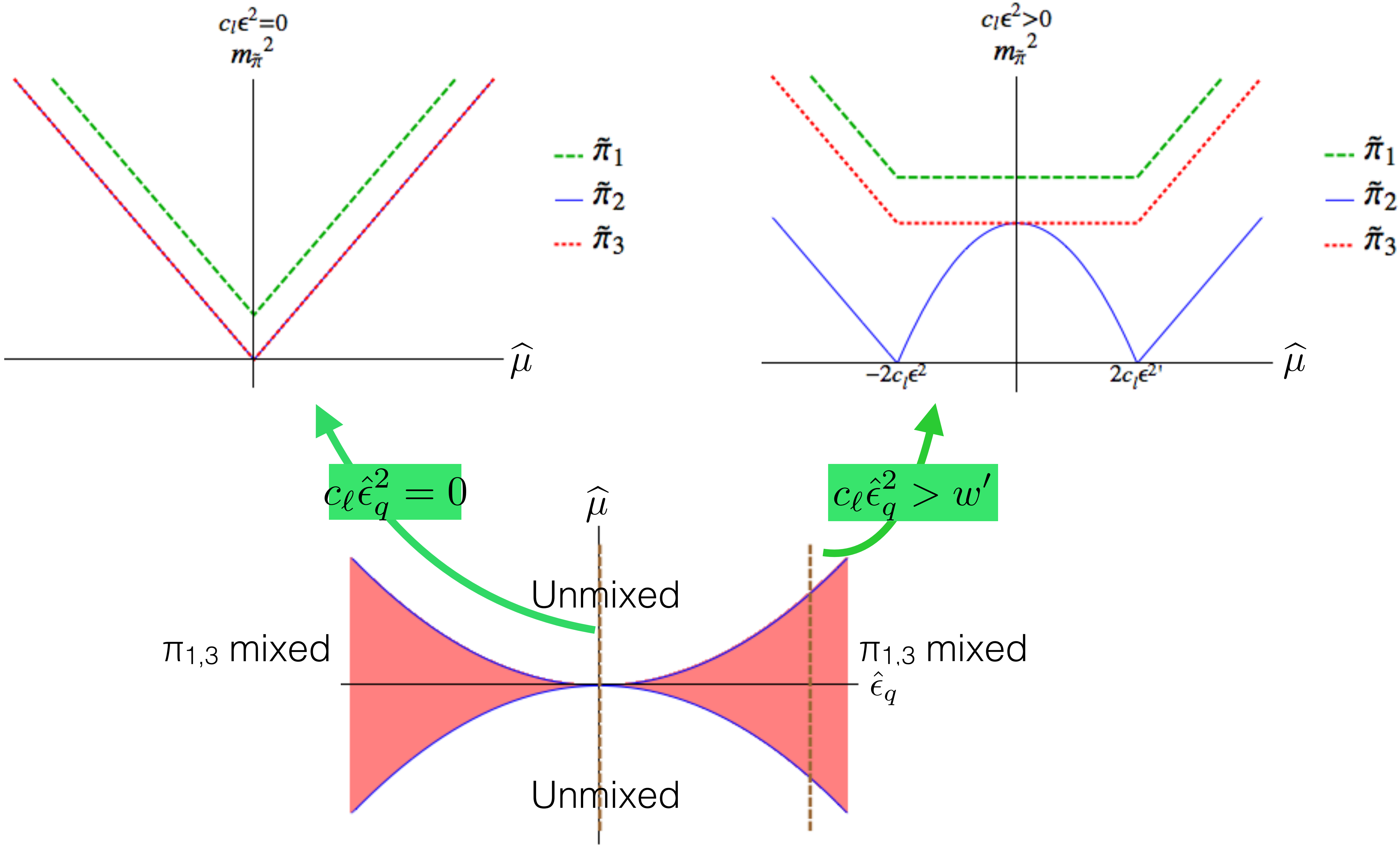
Phase Diagram at maximal twist



First-order Scenario (**w′>0**)

Pion masses at maximal twist

Aoki Scenario (w′<0)



Pion masses at maximal twist

First-Order Scenario (w′>0)