Dynamical $N_f = 3$ lattice QCD simulation project with Wilson-clover quarks

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for CP-PACS/JLQCD collaborations

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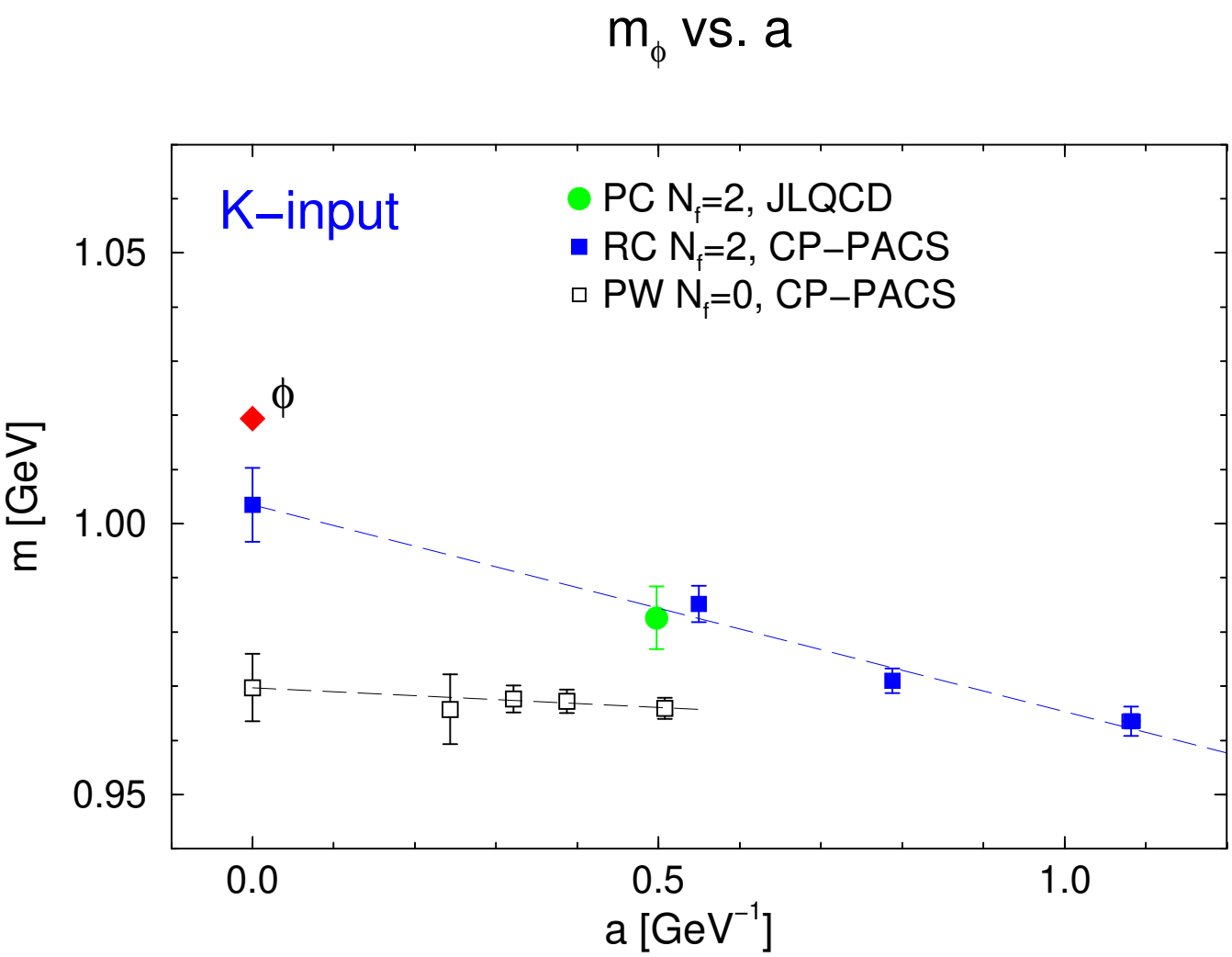
I. Introduction: From quenched to full QCD

CP-PACS collaboration



- m_ϕ(K-input) from quenched QCD disagrees with the experimental value even in the continuum limit (pathology of quenched approximation)

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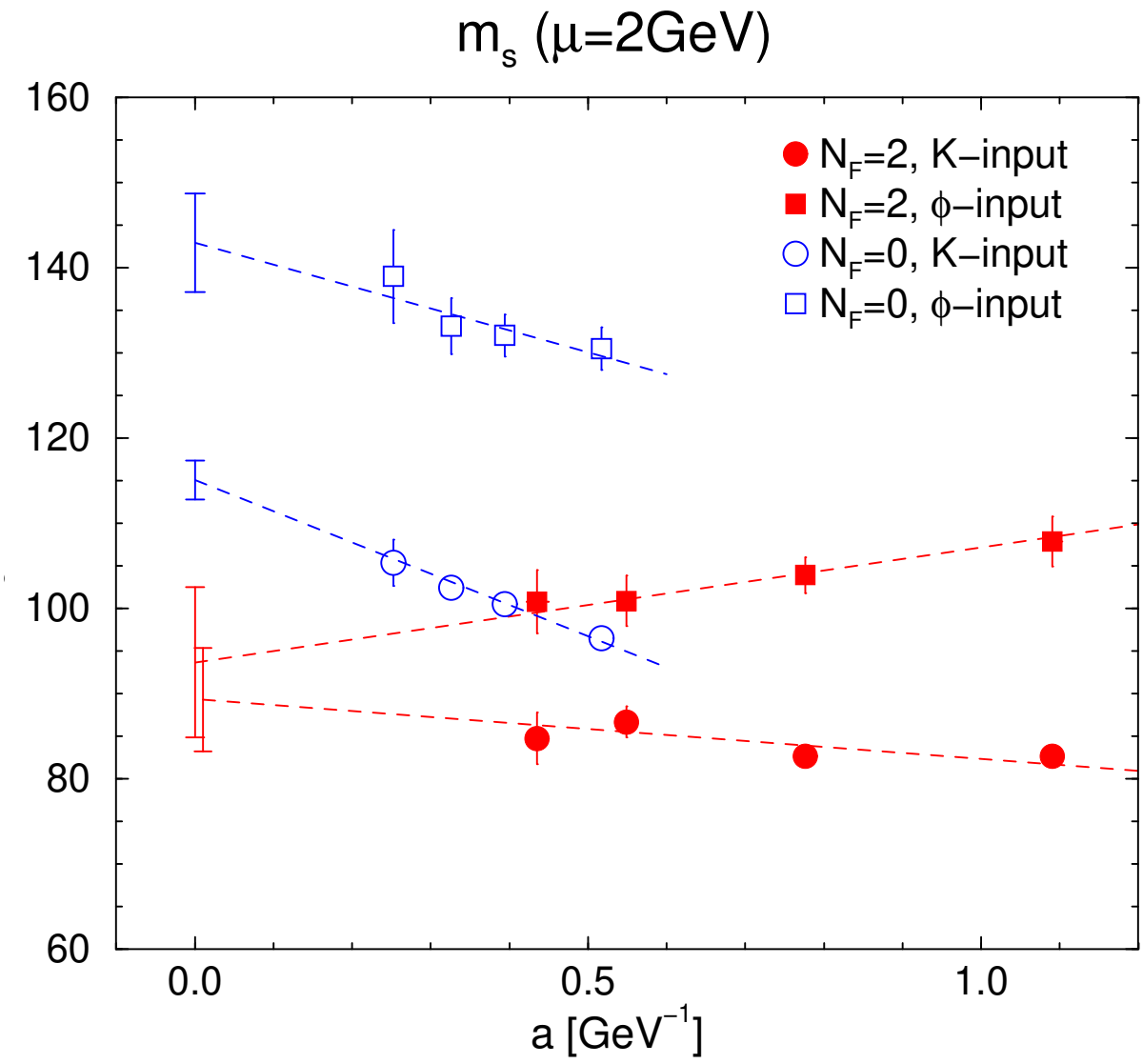
- m_ϕ becomes much closer to the experimental values (two-flavor dynamical quark effect)



- m_s(K-input) and $m_s(\phi$-input) disagree even in the continuum limit
  (pathology of quenched approximation)

$$\Downarrow$$

- m_s(K-input) and $m_s(\phi$-input) seem to agree in the continuum limit
  (two-flavor dynamical quark effect)

Inclusion of dynamical strange quark is the next step

- 2+1 light dynamical quarks
  $\rightarrow$ the correct low energy QCD
- Hadron spectra, strange quark mass
- Weak matrix elements such as $B_K \rightarrow$ CKM matrix
- heavy quark physics $\rightarrow$ CKM matrix

CP-PACS/JLQCD collaborations take the large scale 2+1 flavor dynamical quark simulations as their next main project.

II. Strategy for 2+1 flavors dynamical quark simulations

1. Algorithm
   $m_l \to 0$ extrapolation, while m_s is kept fixed
   - standard Hybrid Monte Carlo (HMC) algorithm for 2 light quarks
   - algorithm for one flavor (the strange quark) $\to$ polynomial HMC (PHMC)

   JLQCD collaboration, hep-lat/0112051

   See later in more detail.

2. Action
   - $O(a)$ improved (clover) quark action with the non-perturbative $c_{\rm SW}$
   - Renormalization Group (RG) improved gauge action
     - 1st order phase transition(lattice artifact) for the clover quark + plaquette gauge actions at $\beta \leq 5.0$ ($a^{-1} \leq 2.6$ GeV)

       JLQCD collaboration, hep-lat/0110088

       See later in more detail.
     - this lattice artifact disappears for the RG gauge action

3. Quark masses
   - 4 values of u, d quark masses ($m_\pi/m_\rho \simeq 0.6 \sim 0.8$) for the chiral extrapolation

     chiral log ?

   - 2 values of the third quark mass for the interpolation to the strange quark mass

4. Lattice spacing and size

- $a^{-1} \simeq (1.0), 1.5, 2.0, (3.0)$ GeV ($a \simeq 0.2 \sim 0.067$ fm) for the continuum extrapolation
- $L \simeq 2.4$ fm to keep the finite size effect for meson masses small enough, but size effect for baryon masses could be larger $\Rightarrow L/a = (12), 16, 24, (32)$

See figures

- Questions
  - $c_{\rm SW}$ can non-perturbatively be determined at $a^{-1} = 1$ GeV ?
  - enough resources to perform simulations at $L/a = 32$?

5. Available computers

- a large part of CPU time will be available for 2+1 simulations
  - CP-PACS at University of Tsukuba, 0.6 Tflops
  - SR800 at KEK, 1.0 Tflops
- a small part of CPU time may be available
  - VP5000 at University of Tsukuba, ?? Tflops
  - Earth Simulator at The Earth Simulator Center, 40 Tflops

6. **Plan of this work**

III. Algorithm for odd numbers of flavor

IV. Non-perturbative determination for $c_{\rm SW}$

V. Some preliminary results

VI. Conclusions and Discussions

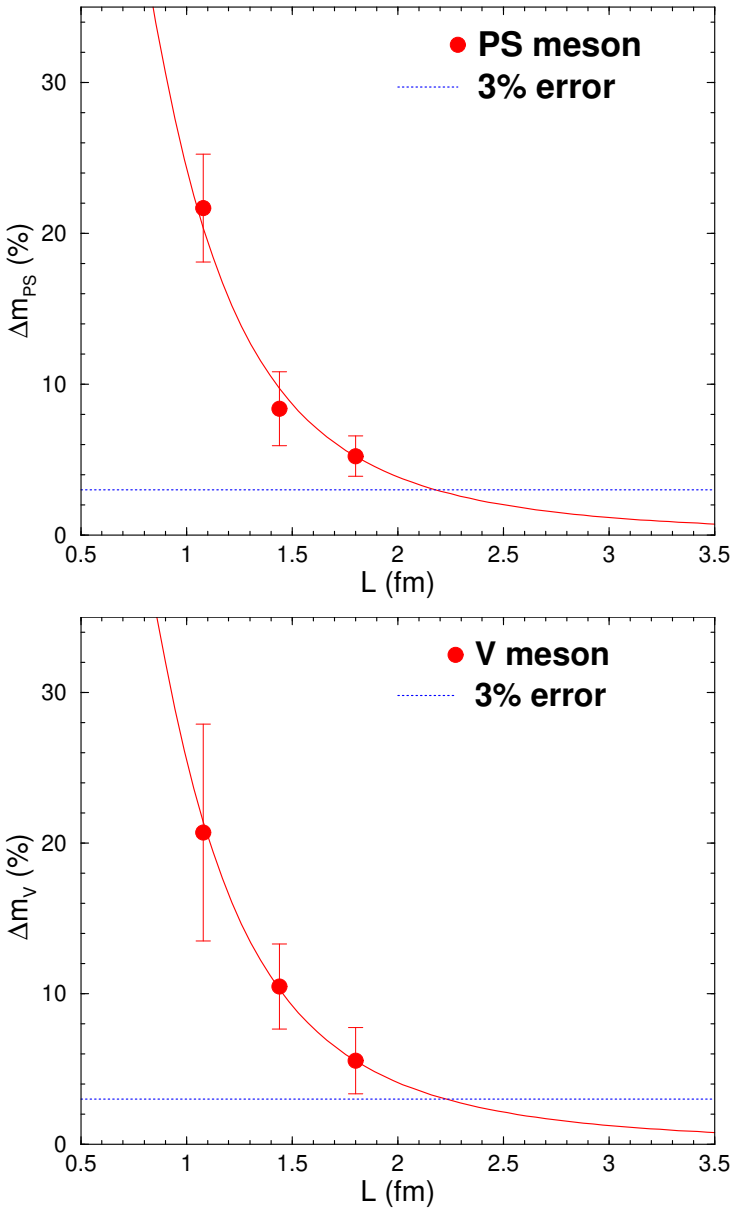
Finite size effect in full QCD

JLQCD collaboration

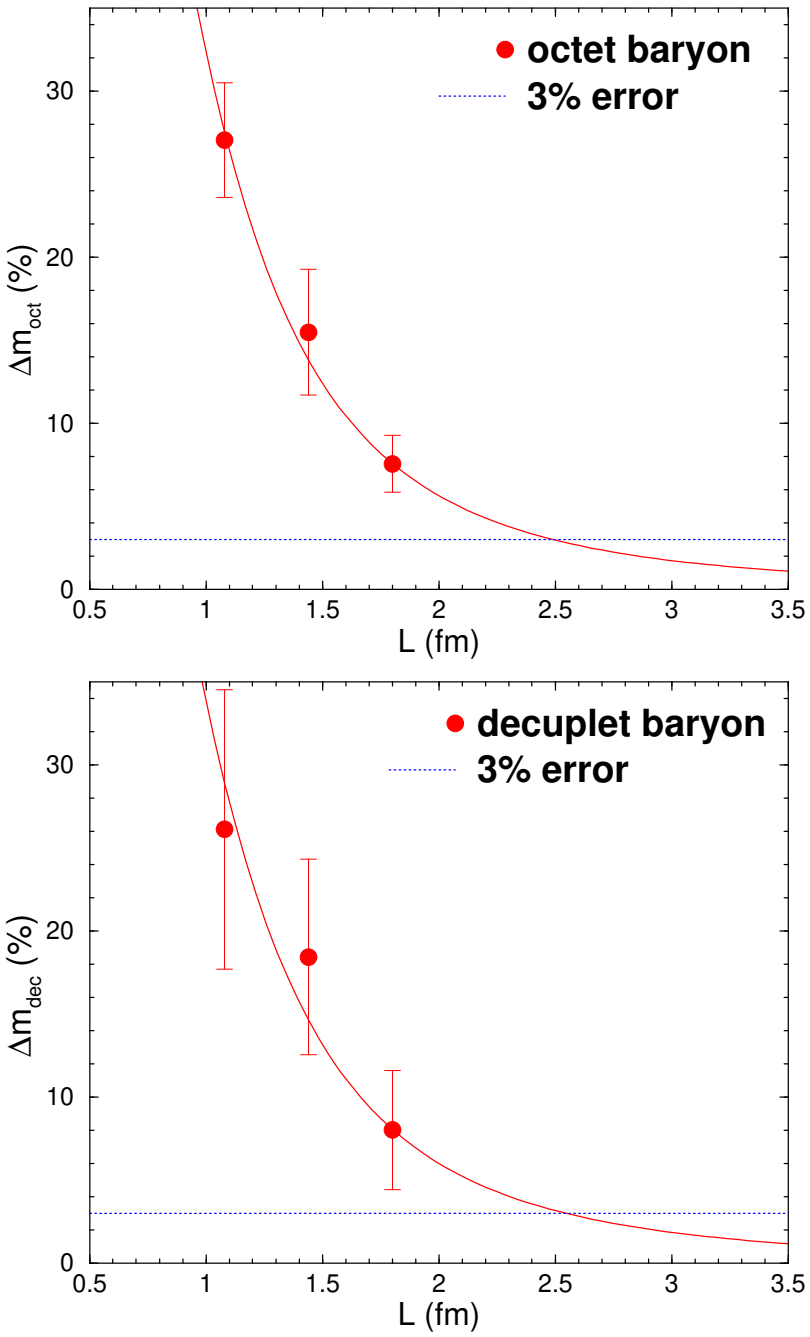
- Plaquette + non-perturbatively (NP) $O(a)$ improved Wilson
- $a^{-1} \simeq 2$ GeV, $m_\pi/m_\rho = 0.60$

$$\Delta m_H(L) \equiv \frac{m_H(L) - m_H(\infty)}{m_H(\infty)} = cL^{-3}$$

Δm_H vs. L (Mesons)



Δm_H vs. L (Baryons)



$\Delta m_H(L) \leq 3\%$

- $La \geq 2.2$ fm for mesons
- $La \geq 2.6$ fm for baryons

III. Algorithm for odd numbers of flavor

Polynomial Hybrid Monte Carlo (PHMC) algorithm

$$Z = \int \mathcal{D}U \, (\det D_1)^{2N_1} \, (\det D_2)^{N_2} \, e^{-S_G(U)}$$

with $D_{1,2}^\dagger = \gamma_5 D_{1,2} \gamma_5$.

even flavors $2N_1$

$$(\det D_1)^{2N_1} = \int \mathcal{D}\phi_1^\dagger \mathcal{D}\phi_1 \exp\left[- \left| D_1^{-N_1} \phi_1 \right|^2 \right]$$

odd flavor N_2

$$\begin{aligned} (\det D_2)^{N_2} &= \left[\frac{\det[D_2 P_{N_{poly}}[D_2]]}{\det P_{N_{poly}}[D_2]} \right]^{N_2} \\ &= \left[\det[D_2 P_{N_{poly}}[D_2]] \right]^{N_2} \int \mathcal{D}\phi_2^\dagger \mathcal{D}\phi_2 \exp\left[- \left| \left(T_{N_{poly}}[D_2] \right)^{N_2} \phi_2 \right|^2 \right] \end{aligned}$$

where

$$\begin{aligned} \det[P_{N_{poly}}[D_2]] &= c \prod_{j=1}^{N_{poly}/2} \det[D_2 - z_j]^\dagger \det[D_2 - z_j] \\ &= \det\left[T_{N_{poly}}[D_2]^\dagger T_{N_{poly}}[D_2] \right], \\ D_2 P_{N_{poly}}[D_2] &\simeq 1. \end{aligned}$$

Here a Metropolis test is needed for the correction factor

$$\det W \equiv \left[\det[D_2 P_{N_{poly}}[D_2]] \right]^{N_2}.$$

A preliminary test for $N_f = 3$

JLQCD collaboration, hep-lat/0110088

Plaquette gauge + $O(a)$ (MF) improved Wilson quark

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1st order phase transition (lattice artifact)

at $\beta \leq 5.0$ ($a^{-1} \leq 2.6$ GeV)

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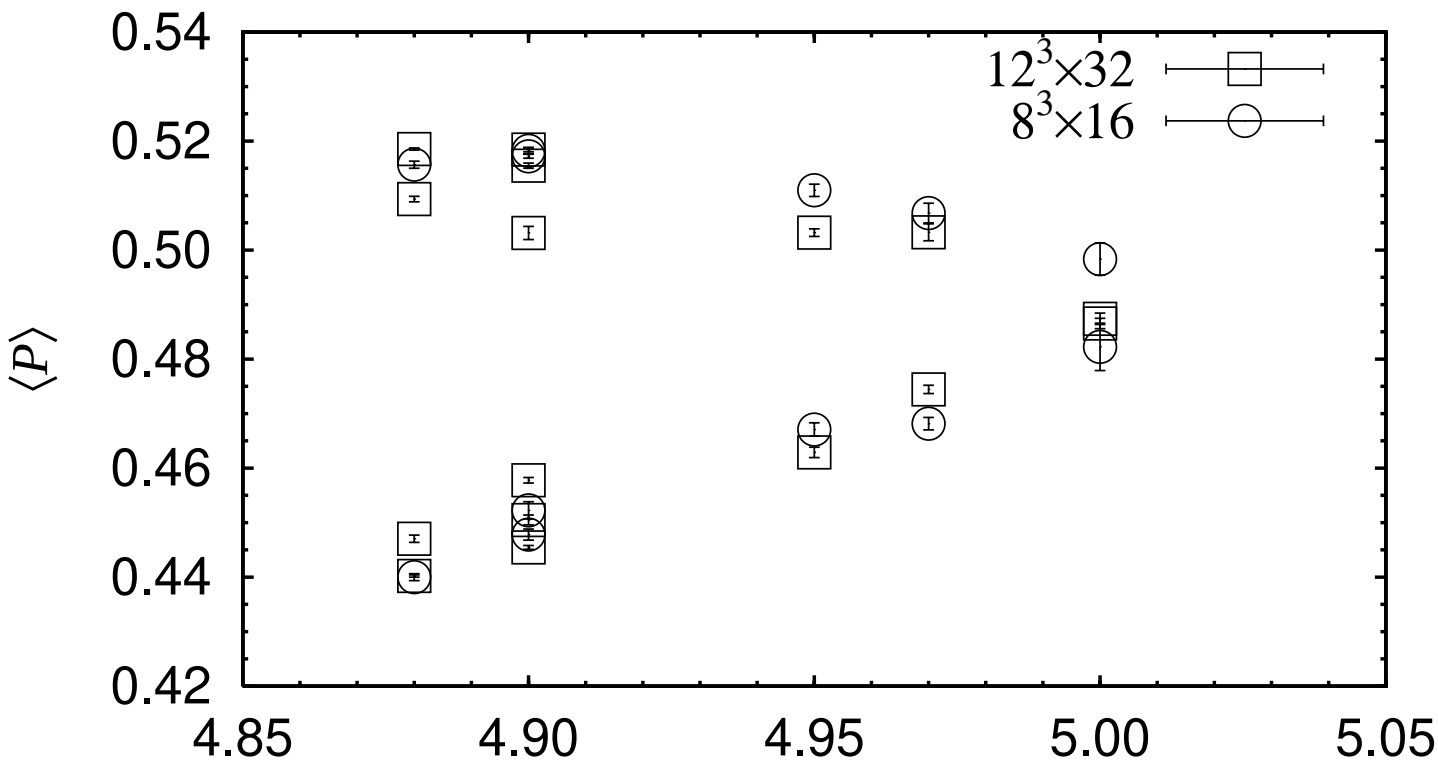
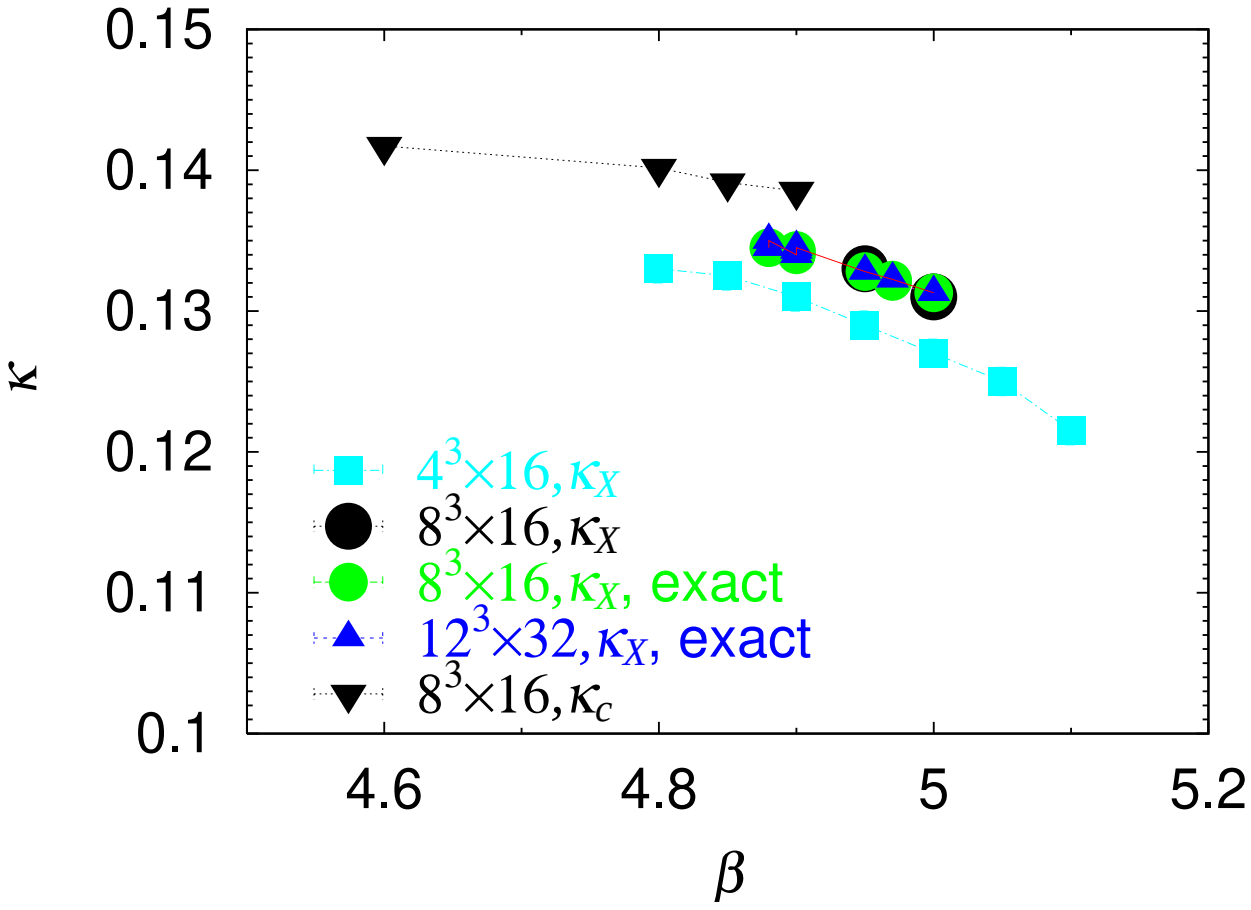
continuum extrapolation from $a^{-1} \simeq 2$ GeV is impossible !

P vs. β at the transition point



Phase structure



This lattice artifact disappears for the RG gauge action.

JLQCD

$\Downarrow$

RG gauge action + $O(a)$ improved Wilson quark action

CP-PACS+JLQCD collaborations

IV. Non-perturbative determination of $c_{\rm SW}$

$O(a)$ improved quark action

$$S_F = a^4 \sum_x \bar{\psi}(x) \left[\gamma_\mu (\nabla^\dagger_\mu + \nabla_\mu) - a \nabla^\dagger_\mu \nabla_\mu + m_0 + c_{\rm SW} \frac{ia}{4} \sigma_{\mu\nu} F_{\mu\nu} \right] \psi(x)$$

$c_{\rm SW}(g_0)$: improvement coefficient

RG improved gauge action

$$S_G = \frac{1}{g^2} \left[c_0 S_{1\times 1} + c_1 S_{1\times 2} \right]$$

with $c_0 + 8c_1 = 1$.

$c_1 = -0.331$: RG improved action by Iwasaki.

$O(a)$ improvement condition from WT identity

tune $c_{\rm SW}$ (and c_A) to satisfy

$$\langle \partial_\mu (A^I_\mu)^a (x_0) \mathcal{O} \rangle = 2m \langle P^a(x) \mathcal{O} \rangle$$

for an arbitrary $\mathcal{O}$, where

$$\begin{aligned}
(A^I_\mu)^a(x) &= A^a_\mu(x) + c_A a \partial_\mu P^a(x) \\
A^a_\mu(x) &= \bar{\psi}(x) \gamma_\mu \gamma_5 \frac{\tau^a}{2} \psi(x) \quad \text{(axial-vector current)} \\
P^a(x) &= \bar{\psi}(x) \gamma_5 \frac{\tau^a}{2} \psi(x) \quad \text{(pseudo-scalar density).}
\end{aligned}$$

Schrödinger Functional (SF) scheme

Alpha Collaboration

- finite volume method on a $L^3 \times T$ lattice
- PBC for space(L^3) and DBC for time(T)
- boundary gauge field at $x_0 = 0,\ T$
  $\rightarrow$ constant background chromo-electric field

quark mass from WT identity

$$m(x_0) = r(x_0) + c_A s(x_0)$$

where

$$r(x_0) \ = \ \partial_0 f_A(x_0)/f_P(x_0), \qquad s(x_0) = a\partial_0^2 f_P(x_0)/f_P(x_0)$$

Modified mass without c_A

$$M(x_0, y_0) \ = \ m(x_0) - s(x_0)\frac{m(y_0) - m'(y_0)}{s(y_0) - s'(y_0)} = r(x_0) - s(x_0)\frac{r(y_0) - r'(y_0)}{s(y_0) - s'(y_0)}$$

Note that $M = m + O(a^2)$ in the improved theory.

Improvement condition for $c_{\rm SW}$

$$\Delta M \equiv M(\frac{3}{4}T, \frac{1}{4}T) - M'(\frac{3}{4}T, \frac{1}{4}T) = \Delta M^0$$

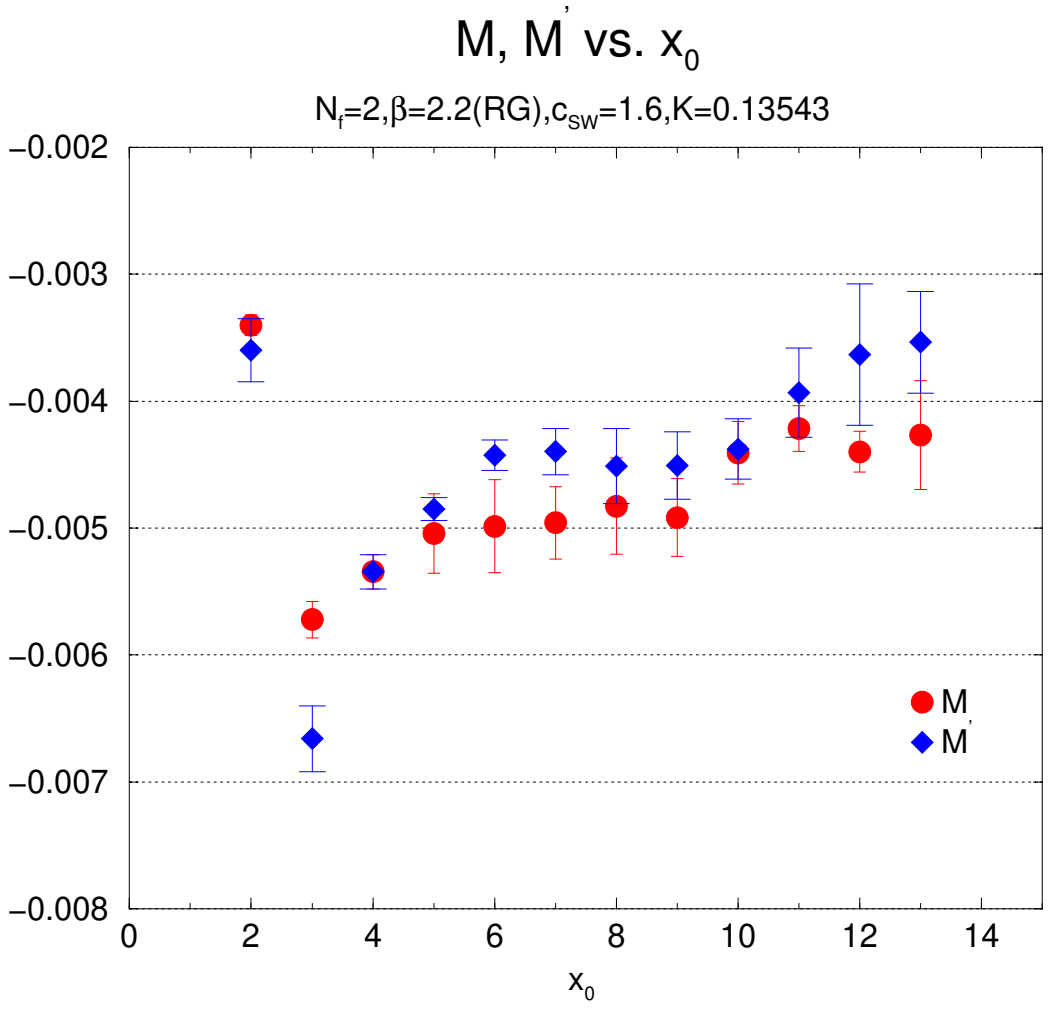
at $M(\frac{1}{2}T, \frac{1}{4}T) = 0$.

ΔM^0 : the value at tree-level on a $L^3 \times T$ lattice.

$L/a = 8$: Alpha's strategy for the plaquette gauge action

$M(x_0, T/4)$ and $M'(x_0, T/4)$ vs. x_0

$N_f = 2$, $\beta = 2.2$(RG), $c_{\rm SW} = 1.6$, $K = 0.13543$

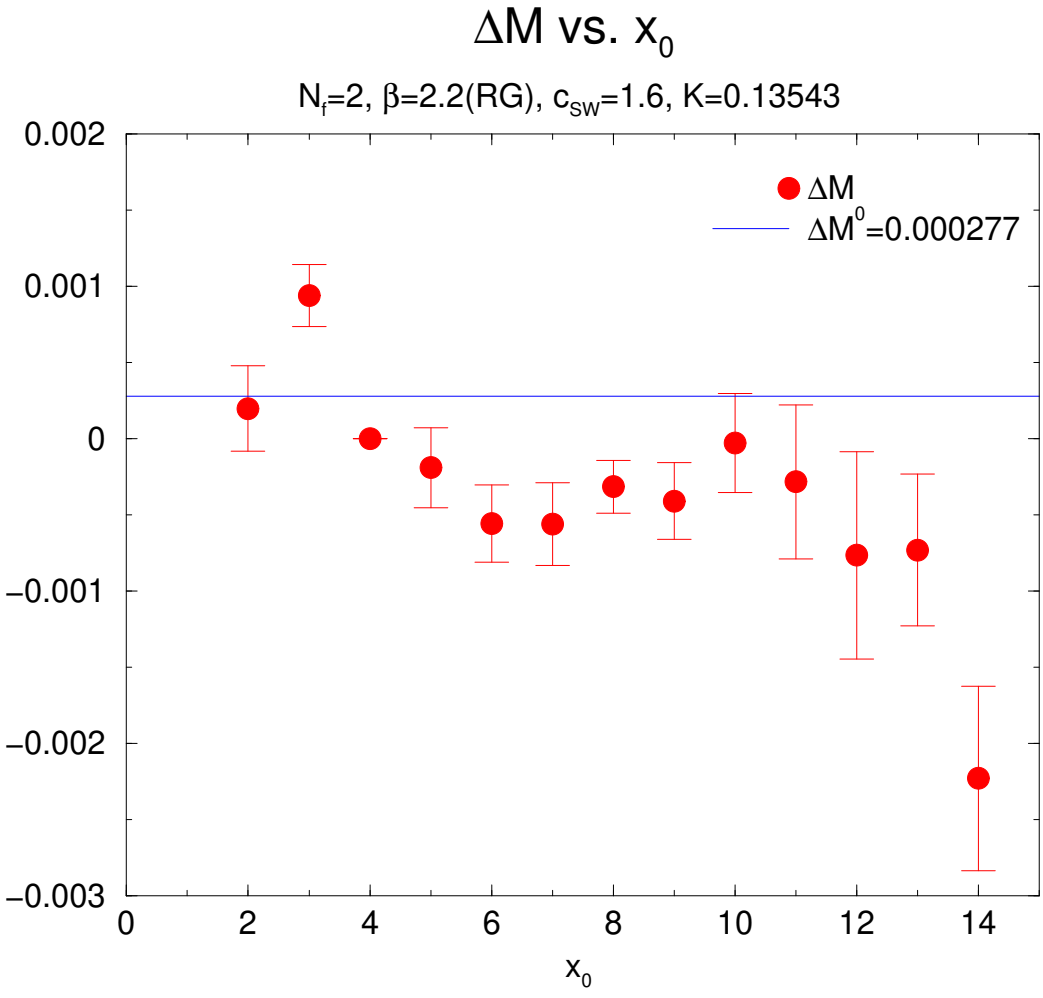


- x_0 dependence is weak away from boundaries
- $M \neq M'$

ΔM vs. x_0

$$\Delta M(x_0) = M(x_0, T/4) - M'(x_0, T/4)$$

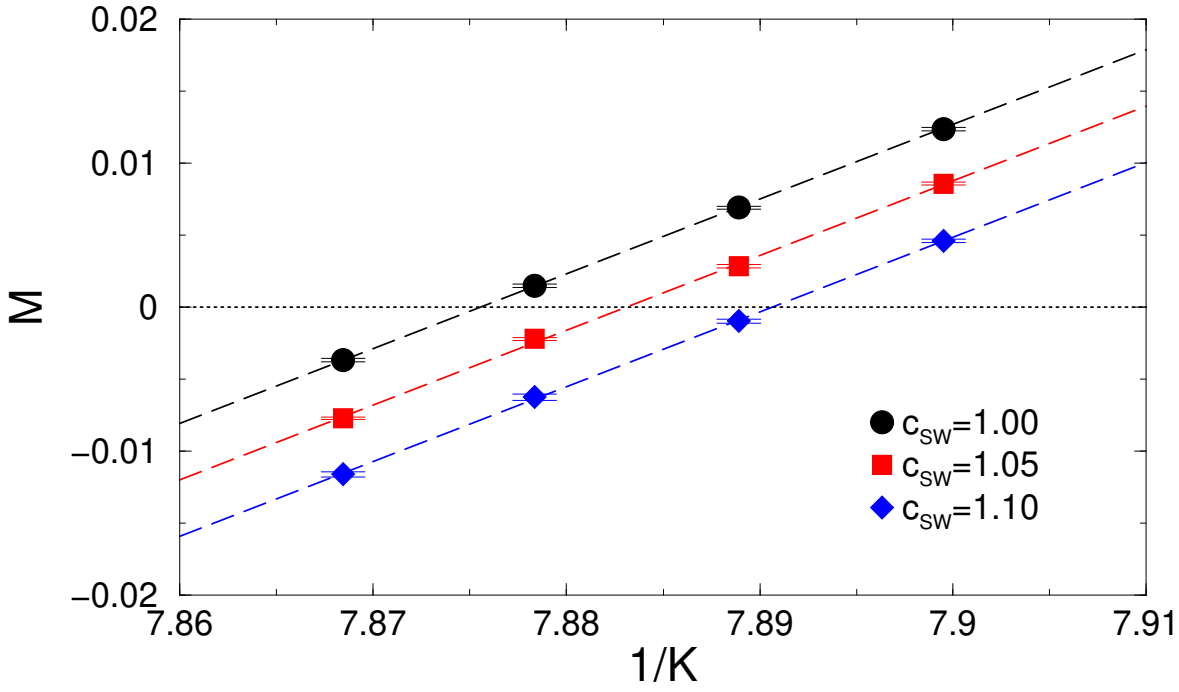
$$N_f = 2,\ \beta = 2.2(\mathrm{RG}),\ c_{\mathrm{SW}} = 1.6,\ K = 0.13543$$

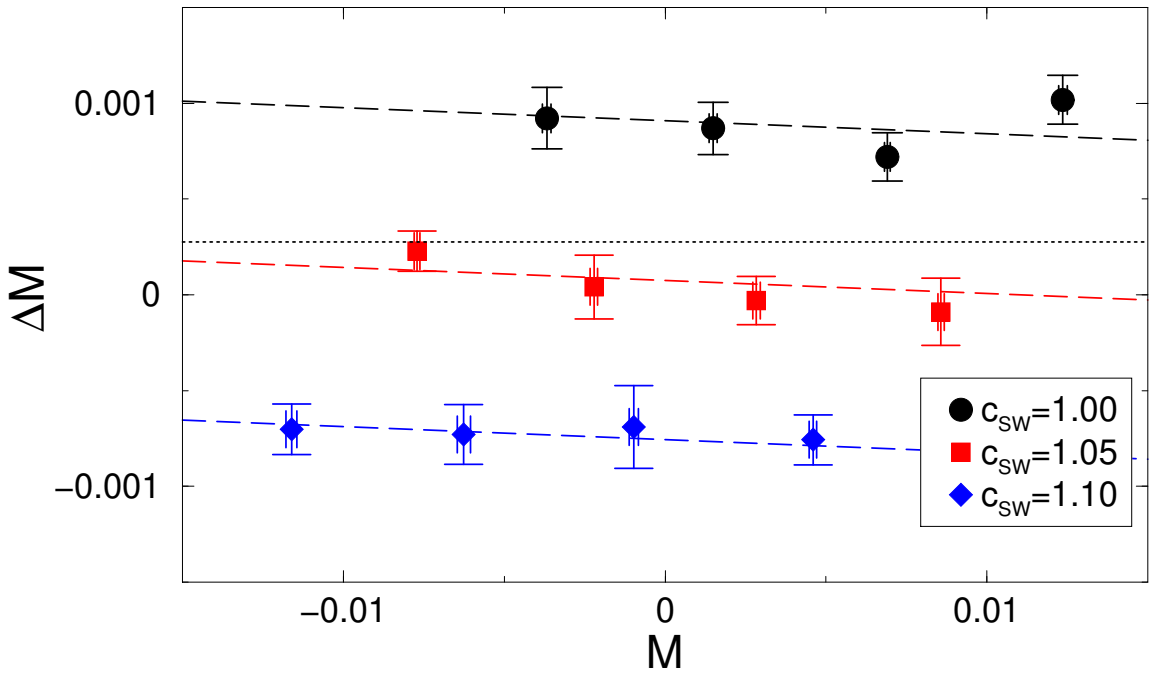


- x_0 dependence is weak away from boundaries
- $\Delta M \neq \Delta M^0$

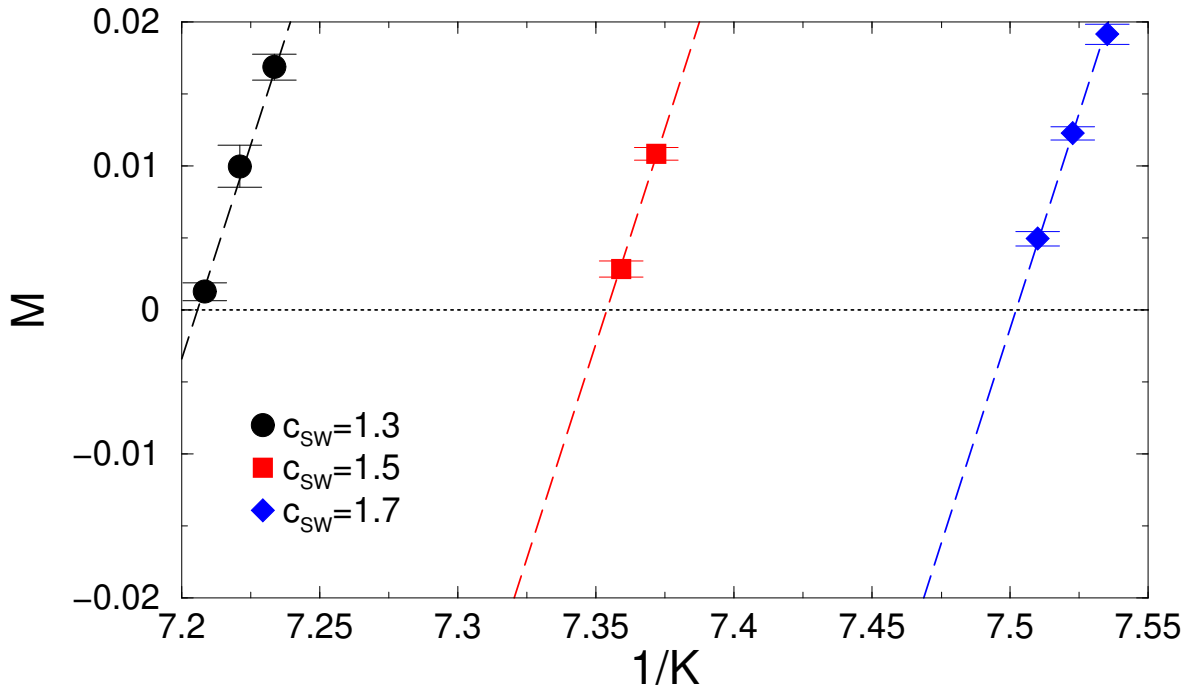
M vs. $1/K$, ΔM vs. M

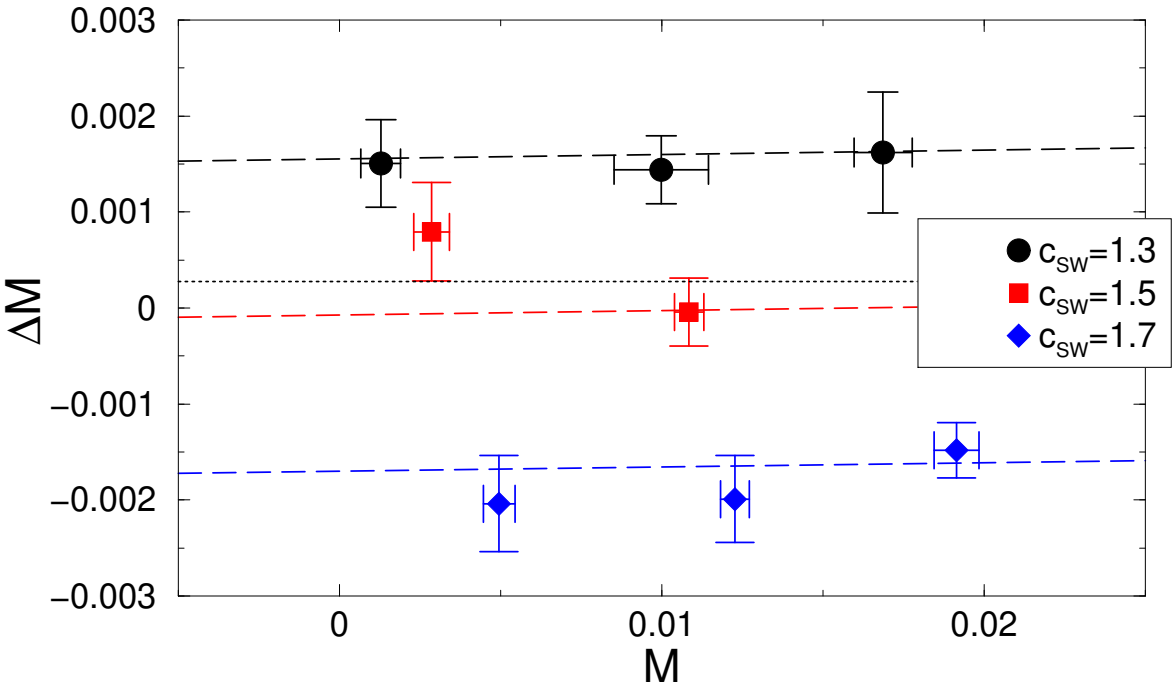
$N_f = 3$, $\beta = 12.0$(RG)





$N_f = 3,\ \beta = 2.2(\mathrm{RG})$





$M \to 0$ extrapolation is needed at strong coupling

Results

Global fits

$$\Delta M = a_0 + a_1 \cdot M + a_2 \cdot c_{\rm SW}, \qquad M = b_0 + b_1 \cdot \frac{1}{K} + b_2 \cdot c_{\rm SW}$$

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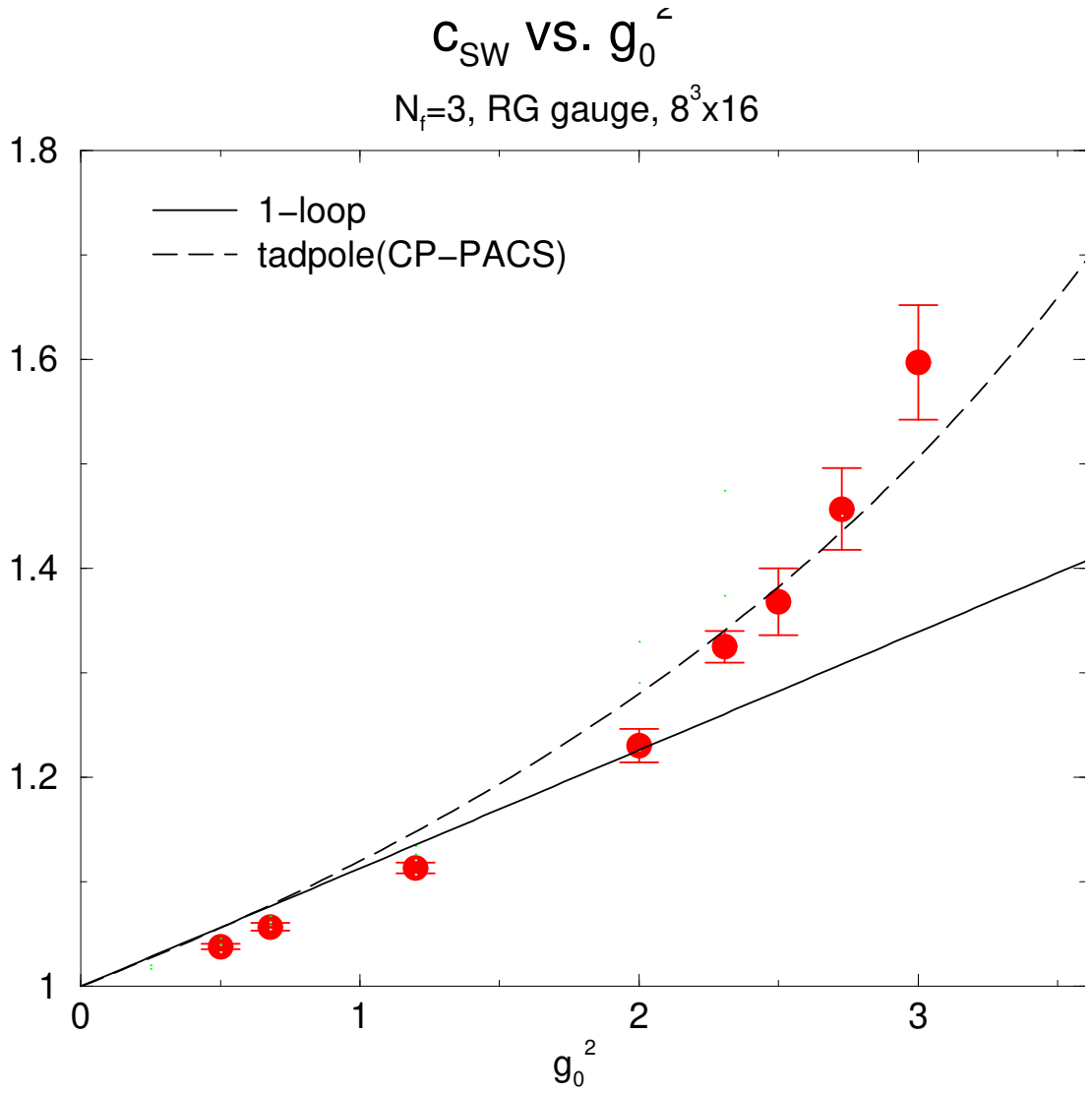
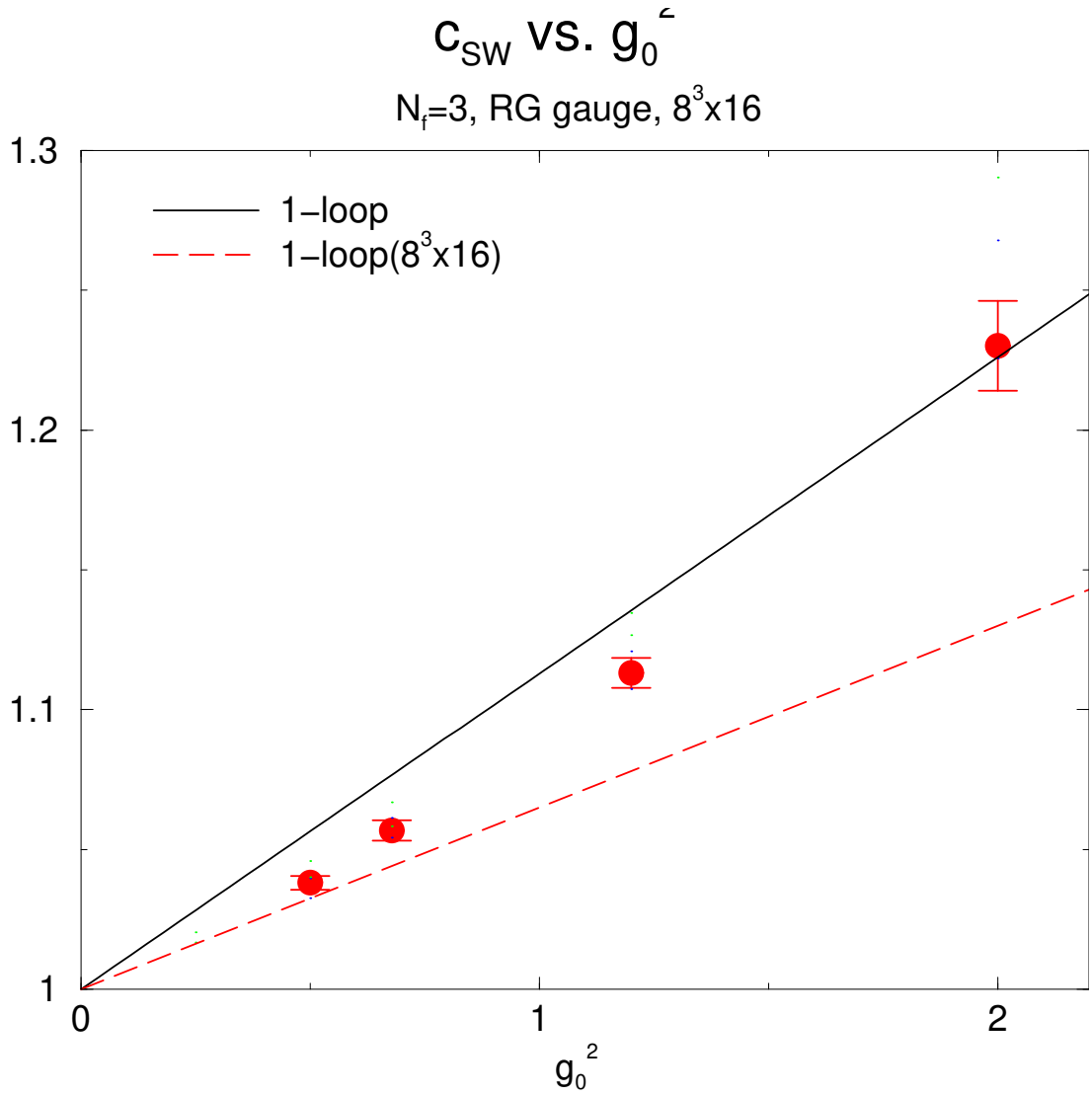
$$c_{\rm SW} = \frac{\Delta M^0 - a_0}{a_2}, \qquad K_c = -\frac{b_1}{b_0 + b_2 \cdot c_{\rm SW}}$$

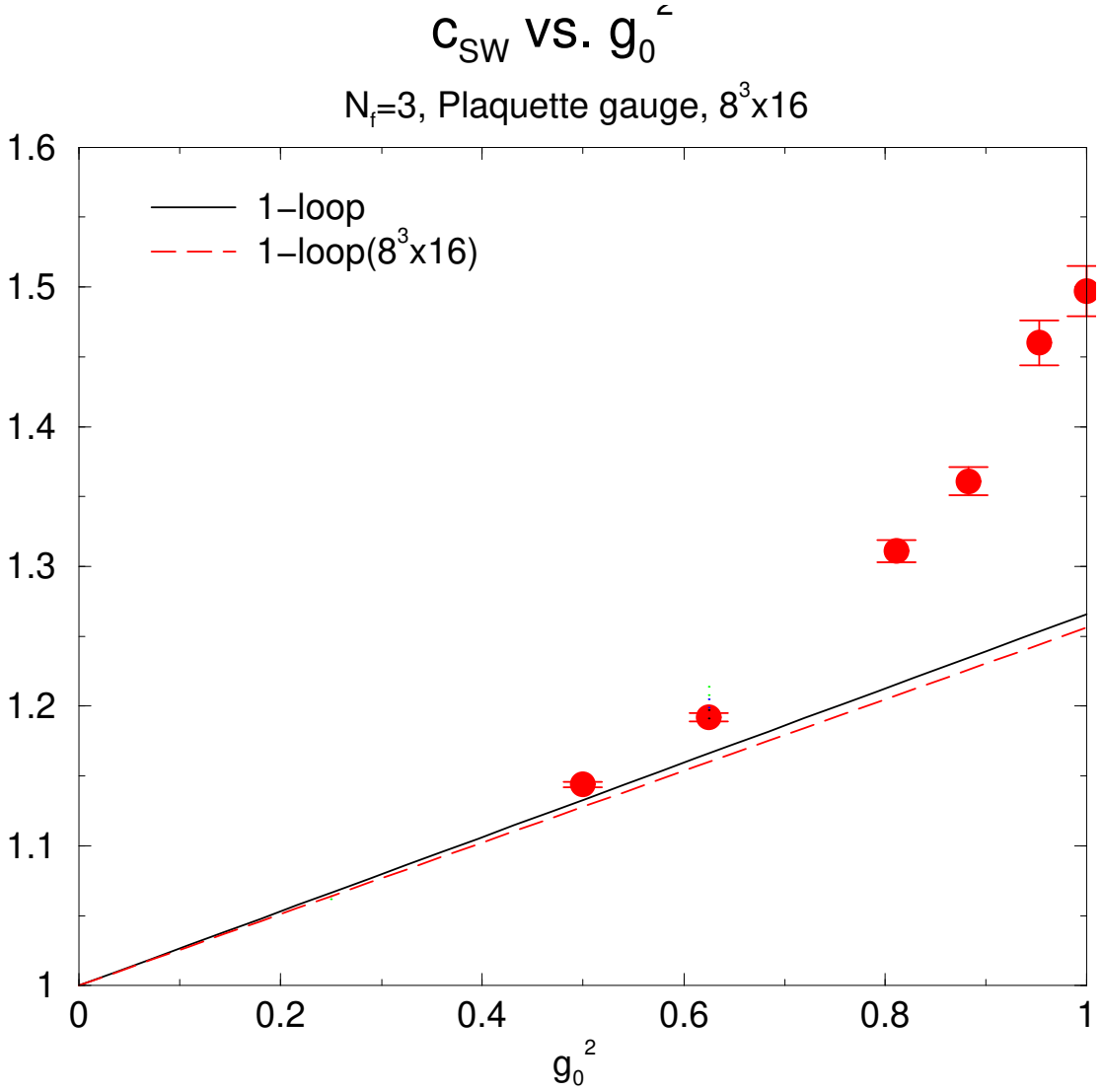


Problem

large $O(g_0^2 a/L)$ correction to $c_{\rm SW}$ at $L/a = 8$



cf. $O(g_0^2 a/L)$ correction is small at $L/a = 8$ for Plaquette action



New strategy to extract $c_{\rm SW}$

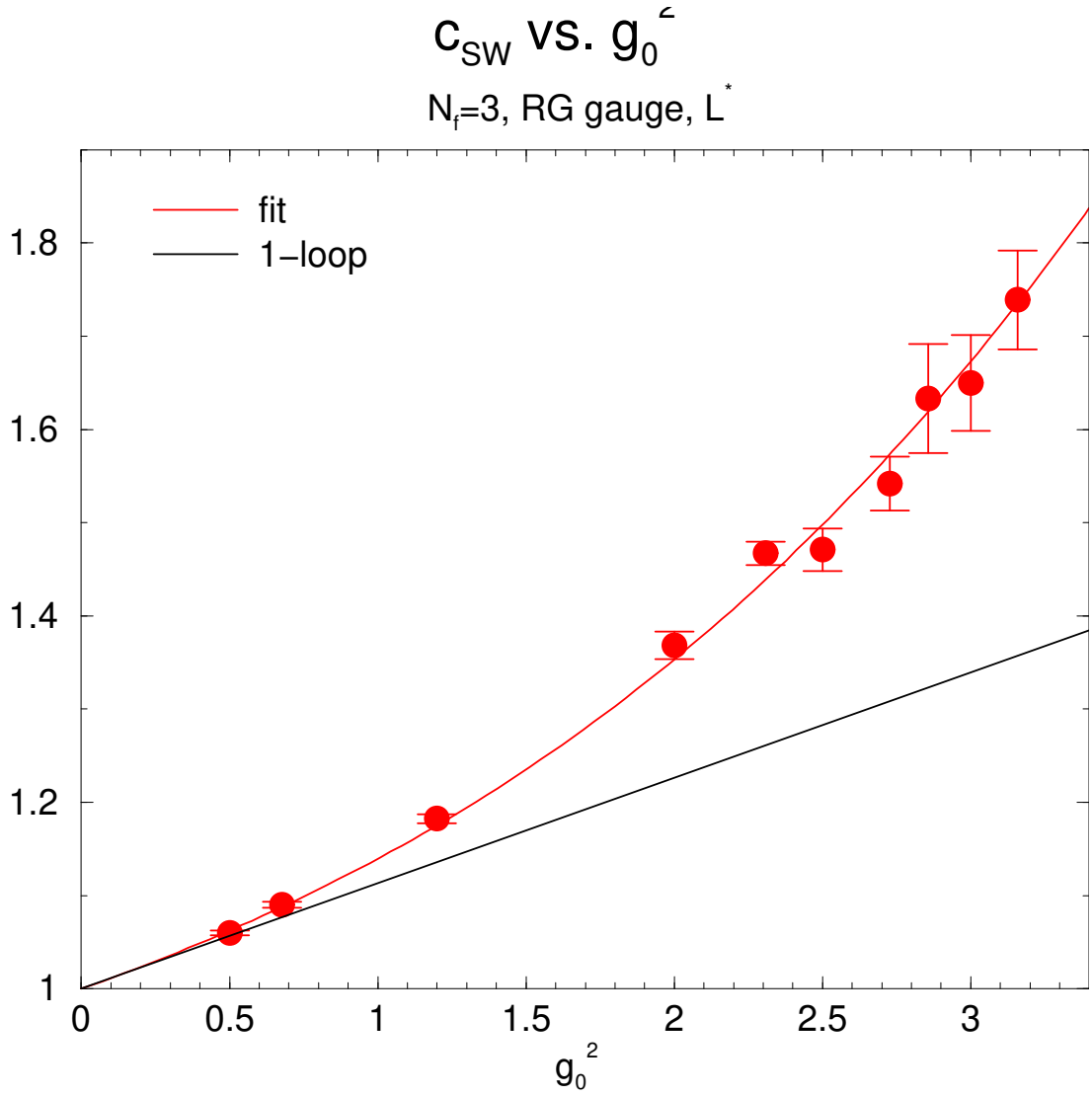
1. try to determine $c_{\rm SW}$ at fixed L^* instead of $L = \infty$
   the difference is $O(a/L^*)$ to $c_{\rm SW}$, so that $O(a^2)$ to observables

2. $c_{\rm SW}$ at $L/a = 8 \Rightarrow c_{\rm SW}$ at L^* by 1-loop estimate

   $$c_{\rm SW}(L^*) = c_{\rm SW}(L/a = 8) + \left[c_{\rm SW}^{1-{\rm loop}}(L^*) - c_{\rm SW}^{1-{\rm loop}}(L/a = 8)\right]$$

3. $L^*/a = 6$ at $\beta = 1.9$ $(g_0^2 = 3.1579)$
   - new data on $6^3 \times 12$ at $\beta = 1.9$
   - L^*/a at other β's (except $\beta = 2.0$) by 2-loop β function
   - $\beta = 2.0$: new data on $6^3 \times 12$ + old data on $8^3 \times 16$ $\Rightarrow c_{\rm SW}$ at $L^*/a = 6.81$ by the interpolation

Final result

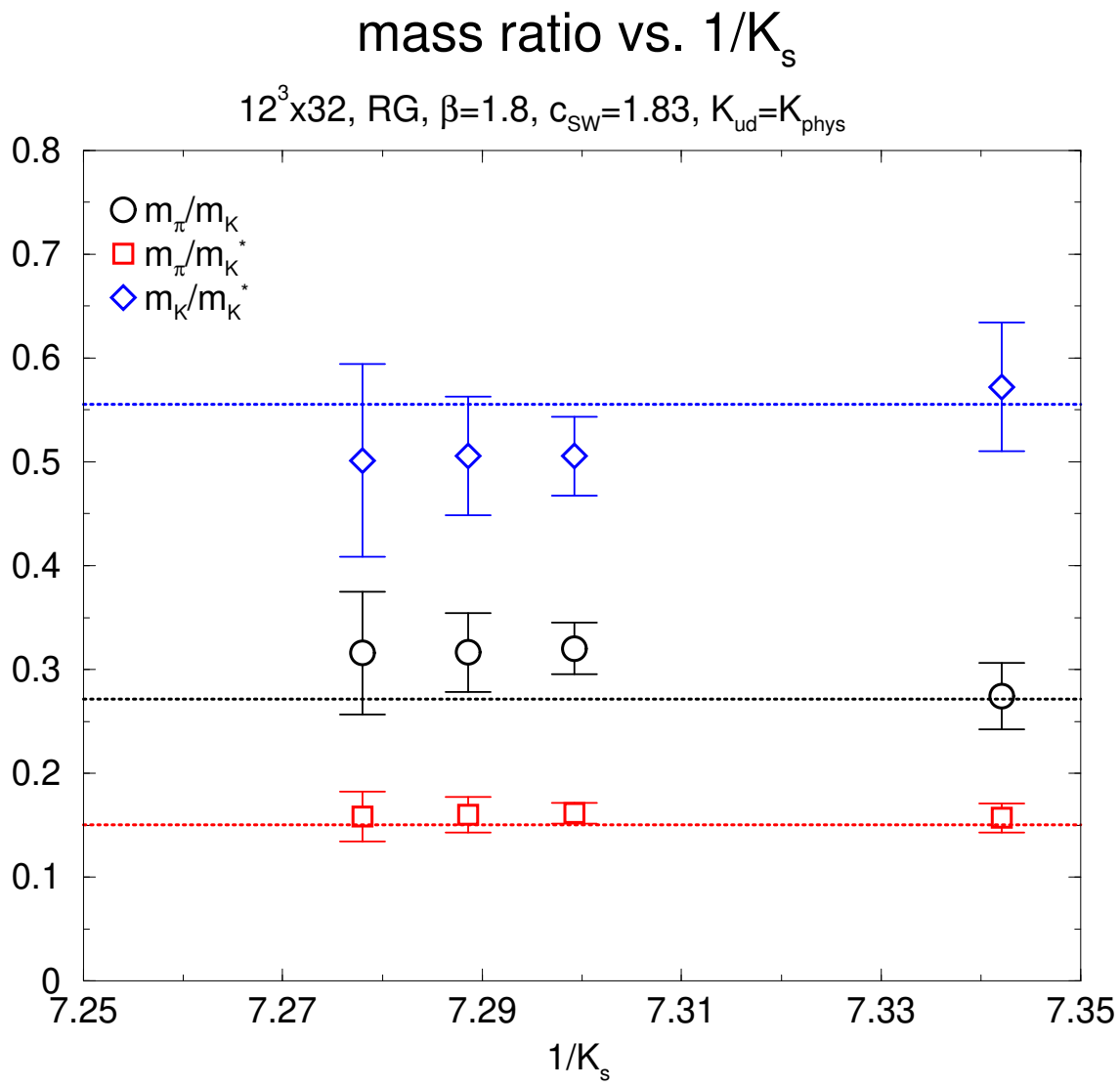


$$c_{\rm SW} = 1 + 0.113 g_0^2 + 0.0209(72) g_0^4 + 0.0047(27) g_0^6$$

V. Some preliminary results

$N_f = 2 + 1$, RG action, $\beta = 1.8$ and $c_{\rm SW} = 1.83$, $12^3 \times 32$

cf. non-perturbative $c_{\rm SW} = 1.785$ by the extrapolation



$a^{-1} = 1.3 \sim 1.5$ GeV from m_ρ

VI. Conclusions and Discussions

1. PHMC algorithm for $N_f = 2+1$ dynamical quarks works well
2. non-perturbative determination of $c_{\rm SW}$ for $N_f = 3$ dynamical quarks with RG gauge action
   - large $O(a/L)$ corrections at $L/a = 8$
   - $c_{\rm SW}$ at L^*, $L^*/a = 6$ at $\beta = 1.9$
   - interpolation formula for $c_{\rm SW}$ at $\beta \leq 1.9$
   - a little extrapolation to $1/a = 1.0 \sim 1.5$ GeV ?
3. Preliminary results of $N_f = 2+1$ simulations at $\beta = 1.8$

4. Spectroscopy(Production runs)
   - $\beta = 1.8$ and $c_{\rm SW} = 1.785$ on $16^3 \times 32$
   - $\beta = 1.9$ and $c_{\rm SW} = 1.715$ on $24^3 \times 48$
   - $\beta = 2.?$ and $c_{\rm SW} = 1.???$ on $32^3 \times 64$?
   - $\beta = 1.7$ and $c_{\rm SW} = 1.868$ on $12^3 \times 24$?
5. Running coupling (SF scheme)
6. Non-perturbative renormalization (SF scheme)