Status of $N_f = 2 + 1 + 1$ flavor twisted mass lattice QCD simulations

Marc Wagner for the ETM Collaboration

Humboldt-Universität zu Berlin, Institut für Physik

Theorie der Elementarteilchen – Phänomenologie/Gittereichtheorie

mcwagner@physik.hu-berlin.de

http://people.physik.hu-berlin.de/∼mcwagner/

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Motivation

- Why lattice QCD simulations with $N_f = 2 + 1 + 1$ dynamical quark flavors?
  - Considering also s and c sea quarks yields a more realistic simulation setup (compared to $N_f = 2$ and $N_f = 2 + 1$).
  - Study the contributions of the dynamical s and c sea quarks to observables; quantify the the so far uncontrolled effect.

Outline

- Introduction to $N_f = 2 + 1 + 1$ Wilson twisted mass lattice QCD.
- Light hadrons.
- Hadrons with s and c valence quarks.

Part 1: introduction to $N_f = 2 + 1 + 1$ Wilson twisted mass lattice QCD.

Twisted mass lattice QCD (1)

- Wilson twisted mass "lattice QCD action" for mass degenerate u/d quarks:

$$S_{u,d} \;=\; \int d^4x \, \bar{\chi}^{(l)} \Big(\gamma_\mu D_\mu + m_{0,l} + i\mu_\mathrm{q}\gamma_5\tau_3 - \frac{a}{2}\Box\Big)\chi^{(l)} .$$

  - $\chi^{(l)} = (\chi^{(u)}, \chi^{(d)})$: twisted basis quark fields.
  - $m_{0,l}$, μ_q: quark masses.
  - τ_3: third Pauli matrix acting in flavor space.
  - In the continuum limit ($a \rightarrow 0$) and after transforming to physical basis quark fields $\psi^{(l)}$ via $\chi^{(l)} = e^{-i\gamma_5\tau_3\omega_l}\psi^{(l)}$, $\omega_l = \mathrm{atan}(\mu_\mathrm{q}/m_{0,l})$ one recovers the standard QCD action for u and d quarks,

$$S_{u,d} \;=\; \int d^4x \, \bar{\psi}^{(l)} \Big(\gamma_\mu D_\mu + m_{u,d}\Big)\psi^{(l)} ,$$

    with $m_{u,d} = \sqrt{(m_{0,l})^2 + (\mu_\mathrm{q})^2}$.

Twisted mass lattice QCD (2)

- Properties of Wilson twisted mass lattice QCD for mass degenerate u/d quarks:

  (+) Automatic $\mathcal{O}(a)$ improvement of observables, when tuned to maximal twist (corresponding to $\omega_l = \pi/2$), i.e. lattice discretization errors appear only quadratically, but not linearly in the small lattice spacing a.

  (+) Moderate computational costs.

  (−) Explicit breaking of isospin I and parity $\mathcal{P}$ by $\mathcal{O}(a)$, i.e. isospin and parity are only approximate symmetries at finite lattice spacing
  $\rightarrow$ different isospin states and $\mathcal{P} = -$ and $\mathcal{P} = +$ states mix, i.e. have to be computed at the same time from the same correlation functions.

Twisted mass lattice QCD (3)

- Wilson twisted mass "lattice QCD action" for s and c quarks:

$$S_{s,c} \quad = \quad \int d^4x \, \bar{\chi}^{(h)} \Big(\gamma_\mu D_\mu + m_{0,h} + i\mu_\sigma \gamma_5 \tau_1 + \mu_\delta \tau_3 - \frac{a}{2}\Box\Big)\chi^{(h)}.$$

  - $\chi^{(h)} = (\chi^{(c)}, \chi^{(s)})$: twisted basis quark fields.
  - $m_{0,h}$, μ_σ, μ_δ: quark masses.
  - τ_1 and τ_3: first and third Pauli matrix acting in flavor space.
  - In the continuum limit ($a \rightarrow 0$) and after transforming to physical basis quark fields $\psi^{(h)}$ via $\chi^{(h)} = e^{-i\gamma_5\tau_1\omega_h}\psi^{(h)}$, $\omega_h = \mathrm{atan}(\mu_\sigma / m_{0,h})$ one recovers the standard QCD action for s and c quarks,

$$S_{s,c} \quad = \quad \int d^4x \, \bar{\psi}^{(h)} \Big(\gamma_\mu D_\mu + \mathrm{diag}(m_c, m_s)\Big)\psi^{(h)},$$

    with $m_{c/s} = \sqrt{(m_{0,h})^2 + (\mu_\sigma)^2} \pm \mu_\delta$.

Twisted mass lattice QCD (4)

- Properties of Wilson twisted mass lattice QCD for s and c quarks::

(+/−) Similar as for the light mass-degenerate u/d doublet ...

(−) ... but instead of isospin breaking explicit heavy flavor breaking by $\mathcal{O}(a)$, i.e. no separate conservation of the number of s and c quarks at finite lattice spacing (only the sum of s and c quarks is conserved)
$\rightarrow$ s and c states mix, i.e. have to be computed at the same time from the same correlation functions.

$N_f = 2+1+1$ ETMC ensembles

- We (the European Twisted Mass Collaboration) have generated/are in the process of generating a variety of ensembles corresponding to
  - different values of the lattice spacing $a \approx 0.061\,\text{fm}\ ,\ 0.078\,\text{fm}\ ,\ 0.086\,\text{fm}$,
  - different values of the light u/d quark masses, which amount to $220\,\text{MeV} \lesssim m_{\text{PS}} \lesssim 510\,\text{MeV}$,
  - different lattice extensions $L^3 \times T = 24^3 \times 48\ ,\ 32^3 \times 64\ ,\ 48^3 \times 96\ ,\ 64^3 \times 128$, which amount to periodic spatial dimensions of extension $1.9\,\text{fm} \lesssim La \lesssim 3.9\,\text{fm}$.
- These ensembles are needed to remove all sources of systematic error (discretization errors, errors due to unphysically heavy u/d quark masses, finite volume corrections) by means of suitable extrapolations.

Hadron masses and decay constants

- Basic principle of determining hadron masses and decay constants via lattice QCD:
  - Compute temporal correlation functions of suitable operators $\mathcal{O}_j$:

    $$\langle\Omega|\Big(\mathcal{O}_j(t)\Big)^\dagger \mathcal{O}_k(0)|\Omega\rangle.$$

  - An operator $\mathcal{O}_j$ is suitable, if the state $\mathcal{O}_j|\Omega\rangle$ has the same quantum numbers as the hadron one intends to investigate.
  - Example: pion.
    * The state $\bar{d}\gamma_5 u|\Omega\rangle$ has isospin $I = 1$, total angular momentum $J = 0$ and parity $\mathcal{P} = -$, i.e. the quantum numbers of the pion.
    * From asymptotic behavior of the temporal correlation function

      $$\langle\Omega|\Big(\bar{d}\gamma_5 u(t)\Big)^\dagger \bar{d}\gamma_5 u(0)|\Omega\rangle =_{t\to\infty} \Big|\langle\text{pion}|\bar{s}\gamma_5 u|\Omega\rangle\Big|^2 e^{-m_\pi t}$$

      one can read of the mass of the pion m_π and its "decay constant" $|\langle\text{pion}|\bar{s}\gamma_5 u|\Omega\rangle|$.

Part 2: light hadrons.

Light hadrons

- The following is a summary of the main results of

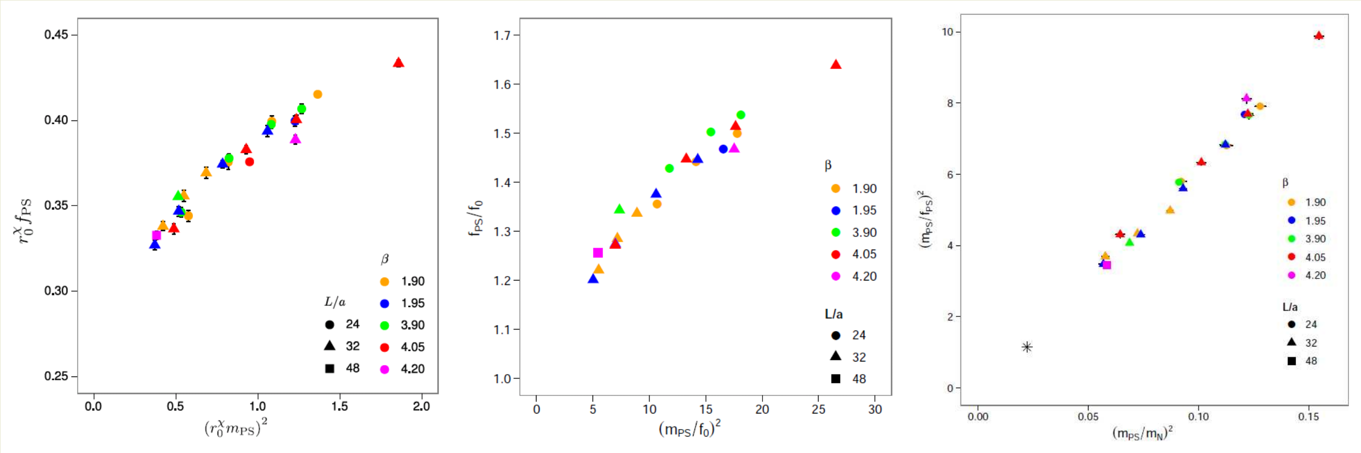
  [R. Baron *et al.*, "Light hadrons from lattice QCD with light (u, d), strange and charm dynamical quarks," JHEP **1006**, 111 (2010), [arXiv:1004.5284 [hep-lat]]].

- Consider observables with u and d valence quarks only:
  - Light charged pseudoscalar mass m_{PS} and decay constant f_{PS} ("pion mass" and "pion decay constant").
  - Nucleon mass m_N (proton mass $=$ neutron mass).

$N_f = 2$ versus $N_f = 2+1+1$ results (1)

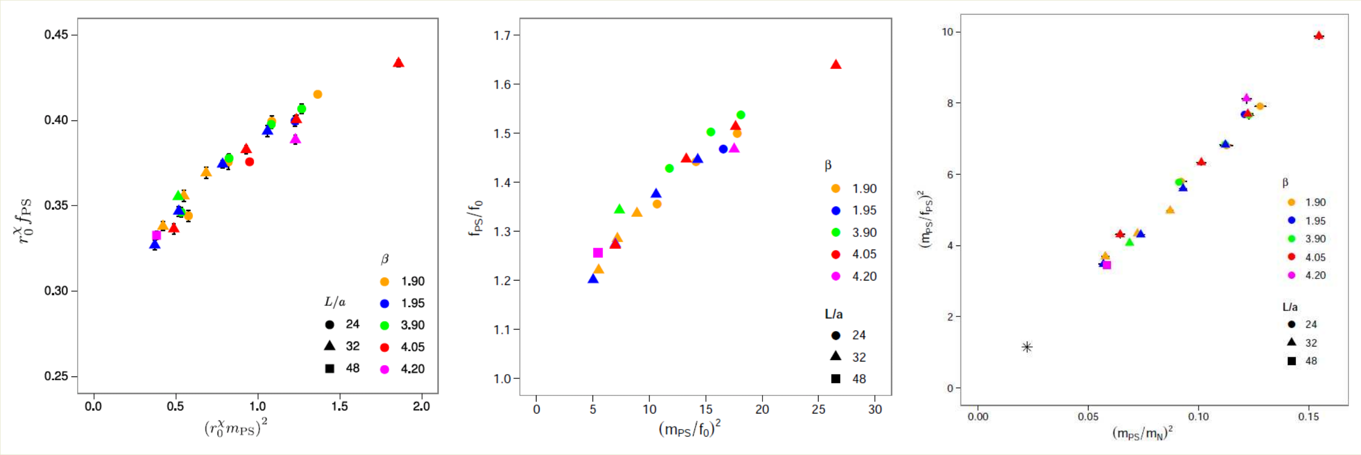
- Consider dimensionless combinations
  $(r_0^\chi m_{\mathrm{PS}})^2$, $r_0^\chi f_{\mathrm{PS}}$, $(m_{\mathrm{PS}}/f_0)^2$, f_{PS}/f_0 , $(m_{\mathrm{PS}}/m_N)^2$, $(m_{\mathrm{PS}}/f_{\mathrm{PS}})^2$.
  - r_0^χ: r_0 in the chiral limit; r_0 is defined via $F_{Q\bar{Q}}(r_0)(r_0)^2 = 1.65$.
  - f_0: light pseudoscalar decay constant in the chiral limit.

- Compare $N_f = 2$ results (three significantly different lattice spacings $a \approx 0.051\,\mathrm{fm}, 0.063\,\mathrm{fm}, 0.079\,\mathrm{fm}$) with $N_f = 2+1+1$ results (two rather similar lattice spacings $a \approx 0.078\,\mathrm{fm}, 0.086\,\mathrm{fm}$)
  $\longrightarrow$ qualitative agreement.



$N_f = 2$ **versus** $N_f = 2+1+1$ **results (2)**

- Conclusions:
  - Discretization errors for $N_f = 2+1+1$ seem to be small.
  - s and c quarks seem to have little effect on the considered light hadronic observables m_{PS}, f_{PS} and m_N.
- To exclude cancellations of discretization errors and effects due to s and c sea quarks, additional $N_f = 2+1+1$ ensembles with smaller lattice spacing(s) need to be investigated.



Chiral perturbation theory (1)

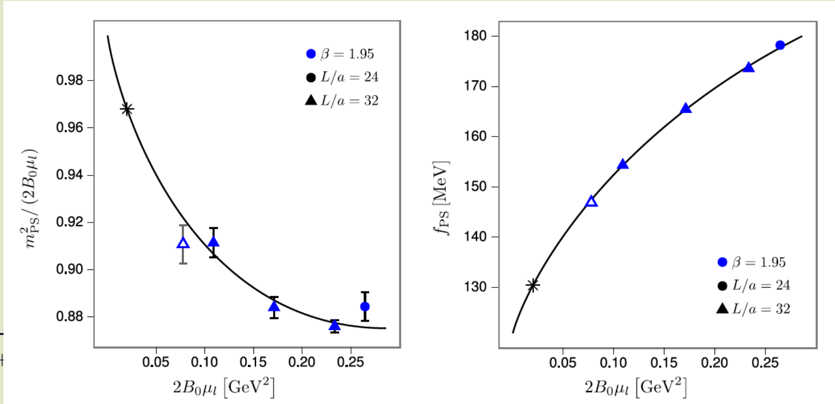
- NLO SU(2) chiral perturbation theory for m_{PS} and f_{PS}:

$$(m_{\text{PS}})^2 \;=\; (m_0)^2\bigg(1 + \frac{(m_0)^2}{32\pi^2(f_0)^2}\ln\Big(\frac{(m_0)^2}{(\Lambda_3)^2}\Big) + \ldots\bigg)\ldots$$

$$f_{\text{PS}} \;=\; f_0\bigg(1 - \frac{(m_0)^2}{16\pi^2(f_0)^2}\ln\Big(\frac{(m_0)^2}{(\Lambda_4)^2}\Big) + \ldots\bigg)\ldots$$

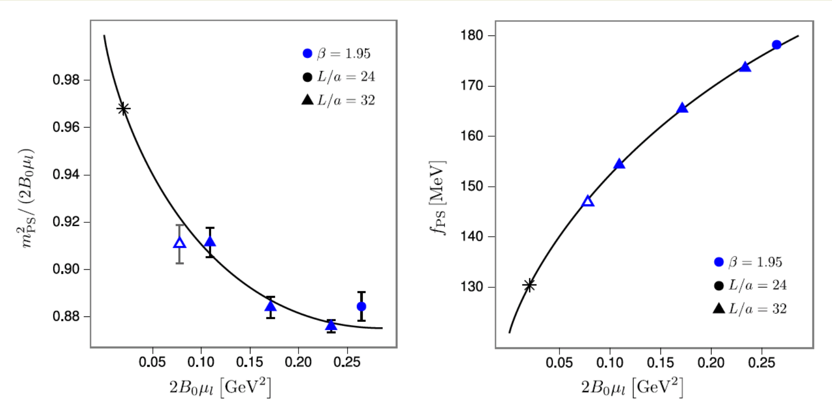
where $(m_0)^2 = 2B_0\mu_l$ and $\bar{l}_{3,4} = \ln((\Lambda_{3,4})^2/(m_\pi)^2)$ ("…" represent terms parameterizing discretization errors and finite volume corrections).

- Fit to lattice results for m_{PS} and f_{PS} obtained with different values of the light quark mass μ_l, the lattice spacing and the spatial volume (fit parameters Λ_3, Λ_4, f_0, B_0).



Chiral perturbation theory (2)

- Scale is set via the physical point $f_{\mathrm{PS}}/m_{\mathrm{PS}} = 130.4(2)\,\mathrm{MeV}/135.0\,\mathrm{MeV}$.
- Results for ensembles with lattice spacing $a \approx 0.078\,\mathrm{fm}$:
  $\bar{l}_3 = 3.70(7)(26)$, $\bar{l}_4 = 4.67(3)(10)$, $f_0 = 121.14(8)(19)\,\mathrm{MeV}$,
  $2B_0\mu_{u,d}/(m_\pi)^2 = 1.032(21)(3)$
  (similar fits to the ensembles with $a \approx 0.086\,\mathrm{fm}$ and simultaneously to both sets of ensembles are used to estimate systematic errors).
- Again good agreement with $N_f = 2$ results,
  $\bar{l}_3 = 3.50(9)(^{+9}_{-30})$, $\bar{l}_4 = 4.66(4)(^{+4}_{-33})$, $f_0 = 121.5(1)(^{+1.1}_{-0.1})\,\mathrm{MeV}$, ...
  and also with results from other collaborations.



Part 3: hadrons with s and c valence quarks.

Mixing of s and c states (1)

- In QCD $n^{(f)} = \#\text{quarks}^{(f)} - \#\text{antiquarks}^{(f)}$ is a separate quantum number for each flavor $f = u, d, s, c, \ldots$
- In Wilson twisted mass lattice QCD the corresponding flavor symmetry is broken by $\mathcal{O}(a)$ for s and c quarks; only $n^{(s)} + n^{(c)}$ is a quantum number.
- Example: kaon (quark content $\bar{s}u$) and D meson (quark content $\bar{c}u$):
  - QCD: kaon has $n^{(s)} = -1$, $n^{(c)} = 0$, D meson has $n^{(s)} = 0$, $n^{(c)} = -1$.
  - Wilson twisted mass lattice QCD: kaon and D meson cannot be distinguished by quantum numbers
    $\rightarrow$ kaon and D meson belong to the same sector of states, i.e. have to be computed at the same time
    $\rightarrow$ since $m_D \gg m_K$, the D meson is a highly excited state in the combined s/c sector ($K(1460)$, ..., $K_0^*(800)$, $K_0^*(1430)$, ..., $K + \pi$, $K + 2 \times \pi$, ... are lighter)
    $\rightarrow$ excited states like the D meson are extremely difficult to compute.

Mixing of s and c states (2)

- Strategy for the computation of s and c observables:
  - Since s and c sea quark masses are tuned to their physical values by requiring that kaon and D meson mass assume their physical values, it is mandatory to compute the kaon and the D meson mass reliably within the **unitary setup** despite the problems caused by heavy flavor mixing.
  - All other s and c observables (f_K, f_D, ..., masses of excited kaons, excited D mesons, D_s mesons, charmonium, baryons containing s and/or c quarks) are/will be computed within a **mixed action setup**:
    * Simulate s and c sea quarks with a non-degenerate Wilson twisted mass doublet.
    * Use a slightly different lattice discretization (Osterwalder-Seiler-like Wilson twisted mass quarks) for valence s and c quarks, where flavor mixing is absent.

$$\Big\langle \mathcal{O}(\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu) \Big\rangle = \int \Big(\prod_f D\chi^{(f)} D\bar{\chi}^{(f)} \Big) DA_\mu \, \mathcal{O}(\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu) e^{-S[\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu]}.$$

Unitary setup: m_K and m_D (1)

- Problem: explicit twisted mass heavy flavor and parity breaking, i.e. the four QCD meson sectors characterized by flavor strange-light/charm-light and parity $-/+$ merge to a single sector in Wilson twisted mass lattice QCD.
- Basic principle:
  - Choose a set of four operators, which excite the kaon, the D meson and their parity partners, but which have only tiny overlap to radial excitations (e.g. $K(1460)$, ...) and multi particle states (e.g. $K + \pi$, ...):

    $$\mathcal{O}_j \quad \in \quad \Big\{\bar{s}\gamma_5 u \; , \; \bar{c}\gamma_5 u \; , \; \bar{s}u \; , \; \bar{c}u\Big\}.$$

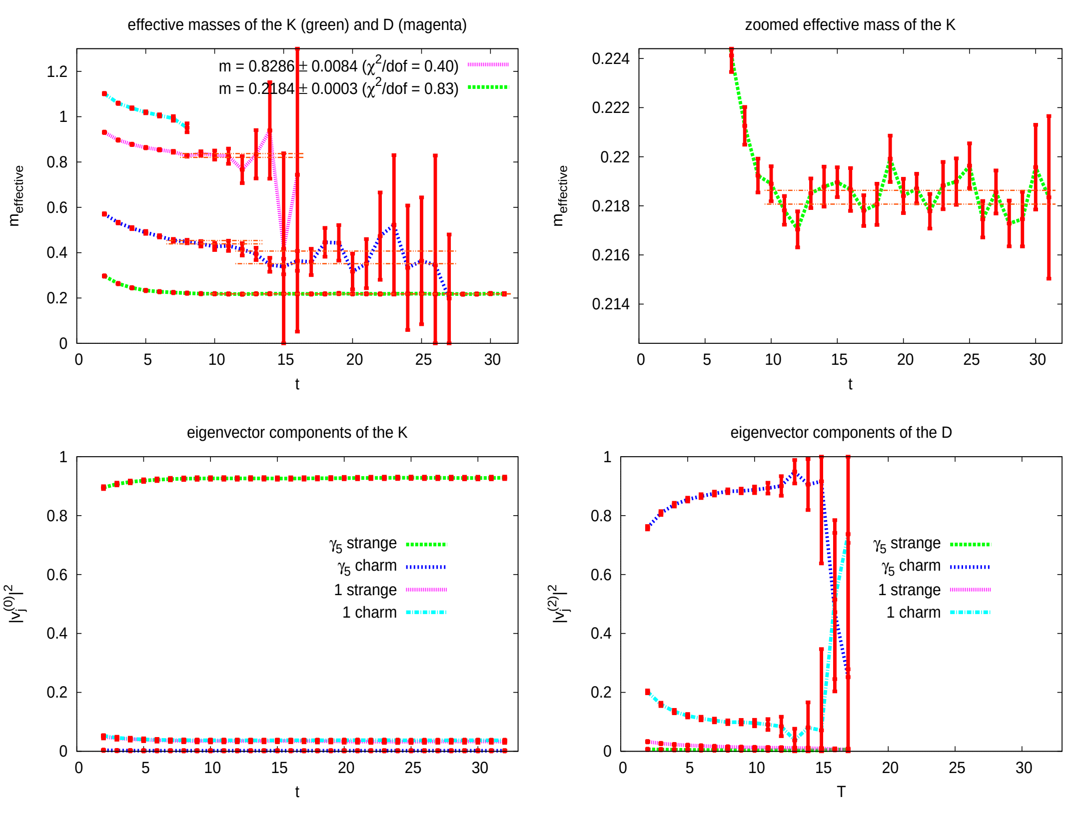
  - Compute the corresponding 4×4 temporal correlation matrix

    $$C_{jk}(t) \quad = \quad \langle\Omega|\Big(\mathcal{O}_j(t)\Big)^\dagger \mathcal{O}_k(0)|\Omega\rangle.$$

  - Diagonalize this correlation matrix at intermediate temporal separations t; the resulting correlators on the diagonal are then approximately proportional to $\exp(-m_K t)$, $\exp(-m_D t)$, $\exp(-m_{K_0^*} t)$, $\exp(-m_{D_0^*} t)$.

Unitary setup: m_K and m_D (2)

- Exemplary plots (ensemble B35.32, i.e. $a \approx 0.078\,\text{fm}$, $m_{\text{PS}} \approx 318\,\text{MeV}$):

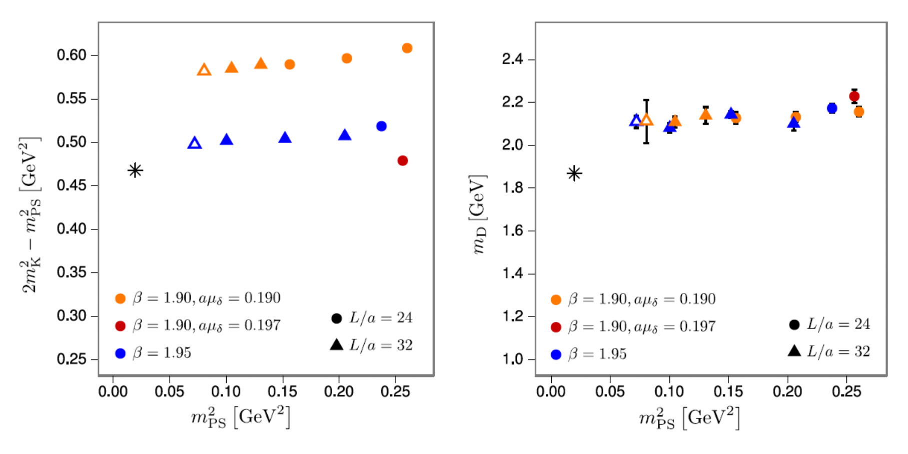


Unitary setup: m_K and m_D (3)

- Control systematic errors induced by mixing of s and c states by
  - monitoring the flavor and parity content of the extracted states,
  - applying three different analysis methods.

    [R. Baron *et al.*,
    "Computing K and D meson masses with $N_f = 2 + 1 + 1$ twisted mass lattice QCD,"
    Comput. Phys. Commun. **182**, 299 (2011) [arXiv:1005.2042 [hep-lat]].

- Summary plots regarding the tuning of the s and c sea quark masses for the ensembles with $a \approx 0.078$ fm and $a \approx 0.086$ fm:



Mixed action setup (1)

- Mixed action setup:

$$\Big\langle \mathcal{O}(\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu) \Big\rangle = \int \Big(\prod_f D\chi^{(f)} D\bar{\chi}^{(f)} \Big) DA_\mu \, \mathcal{O}(\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu) e^{-S[\chi^{(f)}, \bar{\chi}^{(f)}, A_\mu]}.$$

  – Simulate s and c sea quarks with a non-degenerate Wilson twisted mass doublet:

$$S_{s,c} = \int d^4x \, \bar{\chi}^{(h)} \Big(\gamma_\mu D_\mu + m_{0,h} + i\mu_\sigma \gamma_5 \tau_1 + \mu_\delta \tau_3 - \frac{a}{2} \Box \Big) \chi^{(h)}.$$

  – Use Osterwalder-Seiler-like Wilson twisted mass quarks for valence s and c quarks, where flavor mixing is absent:

$$S_{s/c,\mathrm{val}} = \int d^4x \, \bar{\chi}^{(s/c,\mathrm{val})} \Big(\gamma_\mu D_\mu + m_{0,h} \pm i\mu_{s/c,\mathrm{val}} \gamma_5 - \frac{a}{2} \Box \Big) \chi^{(s/c,\mathrm{val})}.$$

- Tune the valence $\mu_{s,\mathrm{val}}$ and $\mu_{c,\mathrm{val}}$ such that the mixed action kaon and D meson masses assume their physical values.

Mixed action setup (2)

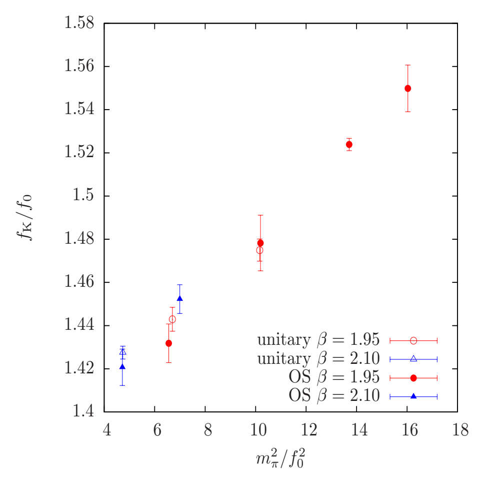
- First step: compute the kaon decay constant f_K within the mixed action setup.

  [F. Farchioni *et al.*, "Pseudoscalar decay constants from $N_f = 2+1+1$ twisted mass lattice QCD," arXiv:1012.0200 [hep-lat]]

- f_K can also be computed rather precisely within the unitary setup.

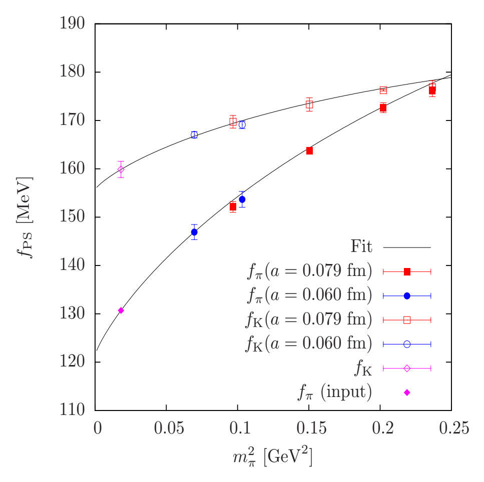
- Comparison of f_K obtained within the mixed action and the unitary setup and for two different values of the lattice spacing $a \approx 0.061\,\mathrm{fm}$ and $a \approx 0.078\,\mathrm{fm}$ $\longrightarrow$ agreement within statistical errors.

- Conclusions:
  - Lattice discretization errors similar for both setups.
  - Lattice discretization errors seem to be small.



Mixed action setup (3)

- Use chiral perturbation theory (finite size corrections included; discretization errors and higher orders ignored at the moment) to determine f_K at the physical point:
  - Preliminary result:
    $f_K/f_\pi = 1.224(13)$, $f_K = 160(2)$ MeV.
  - Agreement with the $N_f = 2$ result:
    $f_K/f_\pi = 1.210(18)$, $f_K = 158(2)$ MeV.
  - Similar computations/analyses for f_D and f_{D_s} underway.



Conclusions

- A variety of ETMC ensembles with $N_f = 2+1+1$ flavors of Wilson twisted mass sea quarks are available for analysis; further ensembles (mainly with small lattice spacings, large volumes, small pion masses) are currently generated and planned.

- Analyses in the light hadron sector (observables m_{PS}, f_{PS}, m_N) yield similar results as for $N_f = 2$, i.e. indicate small lattice discretization errors for $N_f = 2+1+1$ flavors of Wilson twisted mass sea quarks.

- Recently developed analysis methods allow a rather precise determination of m_K and m_D in the unitary setup despite mixing of s and c states, and, therefore, allow a tuning of the s and c sea quark masses to their physical values.

- Further observables containing s and c valence quarks will be computed in a mixed action setup; first results regarding the kaon decay constant f_K computed in this mixed action setup are promising.