Analysis aspects for 2+1+1 flavor twisted mass lattice QCD (K meson mass, D meson mass)

Marc Wagner

Humboldt University Berlin

mcwagner@physik.hu-berlin.de

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

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Outline

- Simulation setup.
- Three methods to determine the mass of the K meson and the mass of the D meson:
  - Generalized eigenvalue problem.
  - Fitting exponentials.
  - Explicit demixing.
- Summary and conclusion.

Simulation setup

- 2+1+1 twisted mass lattice QCD Dirac operators:
  - Degenerate light flavors, quark fields $\chi^{(l)} = (\chi^{(u)}\,,\,\chi^{(d)})$:

$$Q^{(l)} \quad = \quad \gamma_\mu D_\mu + m + i\mu\gamma_5\tau_3 - \frac{a}{2}\Box.$$

  - Non-degenerate heavy flavors, quark fields $\chi^{(h)} = (\chi^{(c)}\,,\,\chi^{(s)})$:

$$Q^{(h)} \quad = \quad \gamma_\mu D_\mu + m + i\mu_\sigma\gamma_5\tau_1 + \tau_3\mu_\delta - \frac{a}{2}\Box.$$

- Simulation setup for results shown in this talk:
  - 220 gauge configurations.
  - $24^3 \times 48$ lattice.
  - $\beta = 1.90$, $\kappa = 0.163335$, $\mu = 0.004$, $\mu_\sigma = 0.15$, $\mu_\delta = 0.19$.

  $\rightarrow$ Pion mass: $am_\pi = 0.1722(25)$.

Goal

- 4 trial states, i.e. 4×4 correlation matrices

$$C_{JJ'}(T) \quad = \quad \langle \phi_J(T) | \phi_{J'}(0) \rangle \quad = \quad \langle \Omega | \mathcal{O}_J(T) (\mathcal{O}_{J'}(0))^\dagger | \Omega \rangle$$

with twisted basis meson creation operators

$$\mathcal{O}_J \quad \in \quad \Big\{ \bar{\chi}^{(d)} \gamma_5 \chi^{(s)} \, , \, \bar{\chi}^{(d)} \gamma_5 \chi^{(c)} \, , \, \bar{\chi}^{(d)} \chi^{(s)} \, , \, \bar{\chi}^{(d)} \chi^{(c)} \Big\}.$$

- Goal: determine $J = 0$ ground state masses for the following mesons.
  - Light-strange, $P = -$ (K meson) ("$\bar{\psi}^{(d)} \gamma_5 \psi^{(s)}$ in the physical basis").
  - Light-charm, $P = -$ (D meson) ("$\bar{\psi}^{(d)} \gamma_5 \psi^{(c)}$ in the physical basis").
  - Light-strange, $P = +$ ("$\bar{\psi}^{(d)} \psi^{(s)}$ in the physical basis").
  - Light-charm, $P = +$ ("$\bar{\psi}^{(d)} \psi^{(c)}$ in the physical basis").
- Main problem: non-trivial relation between physical basis correlation functions and twisted basis correlation functions.

Generalized eigenvalue problem (1)

- Determine low lying eigenstates approximately by solving the generalized eigenvalue problem

$$C_{JJ'}(T_0) v_{J'}^{(n)} \quad = \quad C_{JJ'}(T_0 - 1) v_{J'}^{(n)} \lambda^{(n)}$$

at fixed time T_0 (in this talk: $T_0 = 8$).

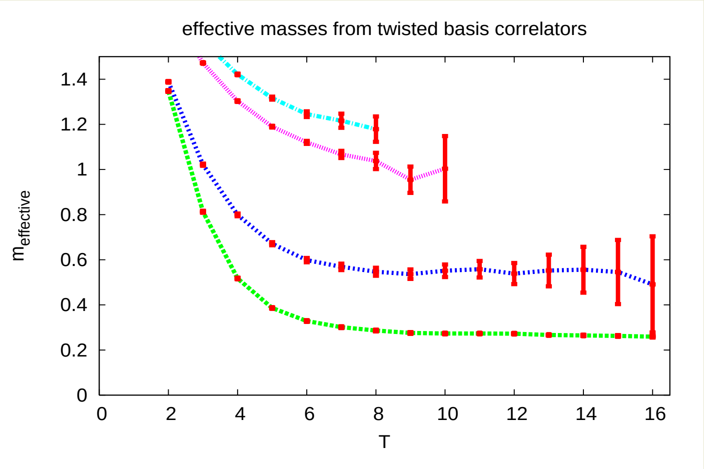
- Effective masses:

$$m_{\mathrm{effective}}^{(n)}(T) \quad = \quad -\log\left(\frac{(v_J^{(n)})^\dagger C_{JJ'}(T) v_{J'}^{(n)}}{(v_J^{(n)})^\dagger C_{JJ'}(T-1) v_{J'}^{(n)}}\right).$$

- Effective mass plateaus correspond to meson masses.

Generalized eigenvalue problem (2)

- Two states can clearly be identified.
- Pros and cons:



(+) Simple: results do not depend on the basis ("no twisted mass knowledge necessary").

(+) Data quality transparent.

(−) Parity and flavor of resulting states not obvious.

(+) Resulting states differ in parity and flavor quantum numbers, i.e. one state for each combination $P = +/P = -$ and strange/charm.
$\rightarrow$ Suited to determine the mass of the D meson.

$*$ Parity and flavor can be assigned from the eigenvectors $v_J^{(n)}$ (assuming $\omega_l \approx \omega_h \approx \pi/2$ and $Z_P/Z_S \approx 1$).

Fitting exponentials (1)

- It can be shown that in the twisted basis parity even correlators are real, whereas parity odd correlators are purely imaginary.

- Ansatz to determine n low lying eigenstates $|j\rangle$:

$$|\phi_J\rangle \equiv \sum_{j=1}^{n} a_j^{(J)} |j\rangle$$

with $a_j^{(J)}$ real, if $|\phi_J\rangle$ is a positive parity trial state, and $a_j^{(J)}$ purely imaginary, if $|\phi_J\rangle$ is a negative parity trial state.

- Correlation matrices in terms of the ansatz:

$$C_{JK}(T) = \langle \phi_J(T) | \phi_{J'}(0) \rangle \equiv \sum_{j=1}^{n} (a_j^{(J)})^* a_j^{(J')} e^{-E_j T} = \tilde{C}_{JJ'}(T).$$

- Determine E_j and $a_j^{(J)}$ by minimizing

$$\chi^2 = \sum_{T=T_{\mathrm{min}}}^{T_{\mathrm{max}}} \sum_J \sum_{K \geq J} \left(\frac{C_{JK}(T) - \tilde{C}_{JK}(T)}{\sigma(C_{JK}(T))} \right)^2 .$$

Fitting exponentials (2)

- Two states can clearly be identified.

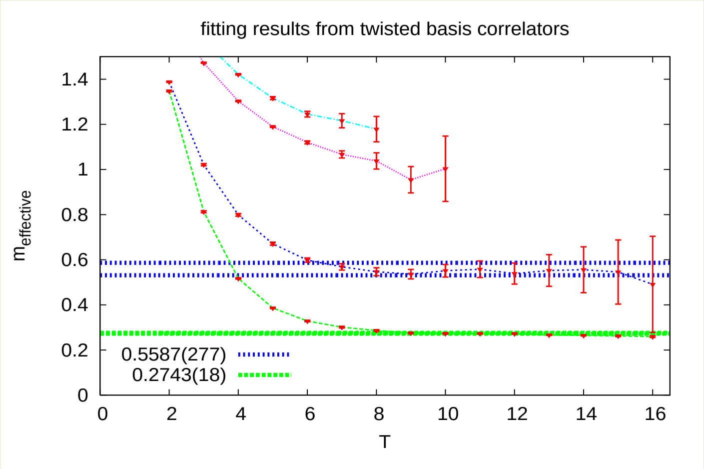
- Pros and cons:

  (+) Statistical analysis more straightforward.

  (−) Parity and flavor of resulting states not obvious.

    (−) **Resulting states do not necessarily differ in parity and flavor quantum numbers.**
    → A determination of the mass of the D meson is difficult.

  $*$ Parity and flavor can be assigned from coefficients $a_j^{(J)}$ (assuming $\omega_l \approx \omega_h \approx \pi/2$ and $Z_P/Z_S \approx 1$).



Explicit demixing (1)

- For each combination $P = +/P = -$ and strange/charm determine the corresponding correlation function in the physical basis.
- Twist rotation for quark fields (in the continuum):

$$\begin{aligned}
\psi^{(l)} &= \frac{1}{\sqrt{2}}\Big(\cos(\omega_l/2) + i \sin(\omega_l/2) \gamma_5 \tau_3\Big) \chi^{(l)} \\
\psi^{(h)} &= \frac{1}{\sqrt{2}}\Big(\cos(\omega_h/2) + i \sin(\omega_h/2) \gamma_5 \tau_1\Big) \chi^{(h)} .
\end{aligned}$$

- Twist rotation for meson creation operators (on the lattice):

$$\begin{pmatrix} \bar{\psi}^{(d)} \gamma_5 \psi^{(s)} \\ \bar{\psi}^{(d)} \gamma_5 \psi^{(c)} \\ \bar{\psi}^{(d)} \psi^{(s)} \\ \bar{\psi}^{(d)} \psi^{(c)} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} c_l c_h & s_l s_h & -i s_l c_h & +i c_l s_h \\ s_l s_h & c_l c_h & +i c_l s_h & -i s_l c_h \\ -i s_l c_h & +i c_l s_h & c_l c_h & s_l s_h \\ +i c_l s_h & -i s_l c_h & s_l s_h & c_l c_h \end{pmatrix} \begin{pmatrix} Z_P \bar{\chi}^{(d)} \gamma_5 \chi^{(s)} \\ Z_P \bar{\chi}^{(d)} \gamma_5 \chi^{(c)} \\ Z_S \bar{\chi}^{(d)} \chi^{(s)} \\ Z_S \bar{\chi}^{(d)} \chi^{(c)} \end{pmatrix} ,$$

where $c_l = \cos(\omega_l/2)$, $s_l = \sin(\omega_l/2)$, $c_h = \cos(\omega_h/2)$, $s_h = \sin(\omega_h/2)$.

Explicit demixing (2)

- Determine the light twist angle ω_l and the heavy twist angle ω_h and the ratio Z_P/Z_S by requiring that the physical basis correlation matrix is diagonal,

$$\begin{aligned}
C^{\text{physical}}_{(\gamma_5,s),(\gamma_5,c)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\gamma_5\psi^{(s)}(T)\Big(\bar{\psi}^{(d)}(0)\gamma_5\psi^{(c)}(0)\Big)^\dagger|\Omega\rangle &= 0 \\
C^{\text{physical}}_{(\gamma_5,s),(1,s)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\gamma_5\psi^{(s)}(T)\Big(\bar{\psi}^{(d)}(0)\psi^{(s)}(0)\Big)^\dagger|\Omega\rangle &= 0 \\
C^{\text{physical}}_{(\gamma_5,s),(1,c)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\gamma_5\psi^{(s)}(T)\Big(\bar{\psi}^{(d)}(0)\psi^{(c)}(0)\Big)^\dagger|\Omega\rangle &= 0 \\
C^{\text{physical}}_{(\gamma_5,c),(1,s)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\gamma_5\psi^{(c)}(T)\Big(\bar{\psi}^{(d)}(0)\psi^{(s)}(0)\Big)^\dagger|\Omega\rangle &= 0 \\
C^{\text{physical}}_{(\gamma_5,c),(1,c)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\gamma_5\psi^{(c)}(T)\Big(\bar{\psi}^{(d)}(0)\psi^{(c)}(0)\Big)^\dagger|\Omega\rangle &= 0 \\
C^{\text{physical}}_{(1,s),(1,c)}(T) &= \langle\Omega|\bar{\psi}^{(d)}(T)\psi^{(s)}(T)\Big(\bar{\psi}^{(d)}(0)\psi^{(c)}(0)\Big)^\dagger|\Omega\rangle &= 0,
\end{aligned}$$

i.e. by minimizing

$$\chi^2 = \sum_{T=T_{\text{min}}}^{T_{\text{max}}} \sum_J \sum_{K\geq J} \left(\frac{C^{\text{physical}}_{JK}(T)}{\sigma(C^{\text{physical}}_{JK}(T))}\right)^2 .$$

Explicit demixing (3)

- Results for different fitting ranges:

fitting range	ω_l	ω_h	Z_P/Z_S	$\chi^2/\mathrm{d.o.f.}$
$2 \leq T \leq 16$	$0.7497(536) \times \pi$	$0.4857(38) \times \pi$	$0.6345(52)$	292.86
$3 \leq T \leq 16$	$0.6204(107) \times \pi$	$0.5007(14) \times \pi$	$0.6380(20)$	25.45
$4 \leq T \leq 16$	$0.6258(94) \times \pi$	$0.5079(12) \times \pi$	$0.6489(19)$	4.23
$5 \leq T \leq 16$	$0.6323(95) \times \pi$	$0.5101(13) \times \pi$	$0.6543(22)$	1.25
$6 \leq T \leq 16$	$0.6366(96) \times \pi$	$0.5105(14) \times \pi$	$0.6566(24)$	0.63

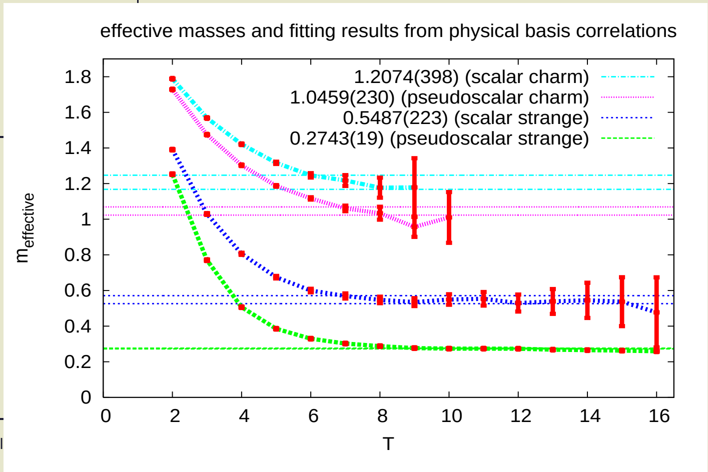
- **Are lattice artifacts responsible?**

Explicit demixing (4)

- Analysis of four individual correlation functions in the physical basis via effective masses and via fitting a single exponential.

- Results for fitting range $6 \leq T \leq 16$:

parity	flavor	m	$\chi^2/\mathrm{d.o.f.}$	particle
$-$	strange	0.2743(19)	0.89	K meson
$-$	charm	1.0459(230)	0.74	D meson
$+$	strange	0.5487(223)	0.04	
$+$	charm	1.2074(398)	0.19	



Explicit demixing (5)

- Rough estimation of meson masses in physical units (assuming $a \approx 0.1\,\mathrm{fm}$):

$$\begin{array}{lcl} am_\pi = 0.1722(25) & \longrightarrow & m_\pi \approx 340\,\mathrm{MeV}\ \text{(PDG: } 139.57018(35)\,\mathrm{MeV}\text{).} \\ am_K = 0.2743(19) & \longrightarrow & m_K \approx 540\,\mathrm{MeV}\ \text{(PDG: } 493.677(16)\,\mathrm{MeV}\text{).} \\ am_D = 1.0459(230) & \longrightarrow & m_D \approx 2100\,\mathrm{MeV}\ \text{(PDG: } 1869.62(20)\,\mathrm{MeV}\text{).} \end{array}$$

- Pros and cons:

  (+) Parity and flavor of resulting states is obvious.

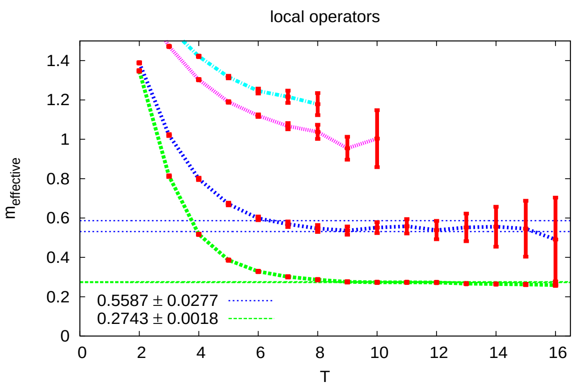
  (+) Determination of the mass of the D meson seems possible with a comparatively small number of contractions.

  (+) Data quality still obvious, when effective masses are computed for individual physical basis correlation functions.

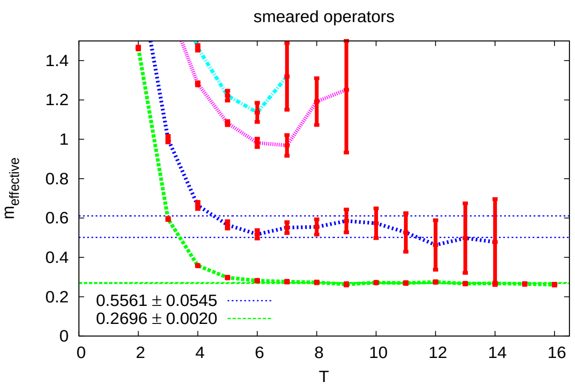
Local versus smeared operators

- **Smearing (fuzzing) increases statistical errors.**

local operators



smeared operators



Summary and conclusion

- Comparison of three analysis methods to determine the mass of the K meson and the mass of the D meson.
  - Generalized eigenvalue problem.
  - Fitting exponentials.
  - Explicit demixing.
- Determination of the mass of the K meson is simple.
  $\longrightarrow$ All three methods agree and yield rather precise results.
- Determination of the mass of the D meson is significantly harder.
  $\longrightarrow$ Use explicit demixing.