The heavy-light sector of $N_f = 2 + 1 + 1$ twisted mass lattice QCD

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Introduction

• Heavy-light sector: mesons made from a “heavy” $s$ or $c$ quark and a light $u$ or $d$ quark.

• Mainly $K$ (e.g. $\bar{s}u$, $J^P = 0^-$) and $D$ (e.g. $\bar{c}u$, $J^P = 0^-$).

• Problems arise in particular, when considering charmed mesons (the $D$), because of twisted mass flavor breaking.
Outline

- $N_f = 2 + 1 + 1$ tm lattice QCD.
- $m(K)$ and $m(D)$.
  - A. Generalized eigenvalue problem.
  - B. Fitting exponentials.
  - C. Parity and flavor restoration
- Optimization of operators.
- Decay constants $f_K$ and $f_D$.
- Vector mesons $K^*$ and $D^*$.
- Status at “Lattice 2009”.
- Mixed action OS setup.
- Conclusions.
\[ N_f = 2 + 1 + 1 \text{ tm lattice QCD} \] (1)

- Dirac operator of the mass degenerate light doublet:

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

- Dirac operator of the mass split heavy doublet:

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

- Because of the Wilson term \(-(a/2)\Box\), parity is not a symmetry and the heavy flavors cannot be diagonalized

→ instead of the four sectors \((s, -), (s, +), (c, -), (c, +)\) there is only a single “combined” sector \((s/c, -/+)\) in twisted mass lattice QCD.
\[ N_f = 2 + 1 + 1 \text{ tm lattice QCD} \ (2) \]

- Twist rotation (in the continuum):

\[
\begin{pmatrix}
\psi^{(u)} \\
\psi^{(d)}
\end{pmatrix}
= \exp \left( i \gamma_5 \tau_3 \omega_l / 2 \right)
\begin{pmatrix}
\chi^{(u)} \\
\chi^{(d)}
\end{pmatrix}
\]

\[
\begin{pmatrix}
\psi^{(s)} \\
\psi^{(c)}
\end{pmatrix}
= \exp \left( i \gamma_5 \tau_1 \omega_h / 2 \right)
\begin{pmatrix}
\chi^{(s)} \\
\chi^{(c)}
\end{pmatrix}
\].

- Typically we use the twisted basis meson creation operators

\[
O_j \in \left\{ \bar{\chi}^{(d)} \gamma_5 \chi^{(s)}, \bar{\chi}^{(d)} \gamma_5 \chi^{(c)}, \bar{\chi}^{(d)} \chi^{(s)}, \bar{\chi}^{(d)} \chi^{(c)} \right\},
\]

to access the \( J = 0 \) \((s/c, -/+\)) sector (the \( K \) and the \( D \)).
$N_f = 2 + 1 + 1$ tm lattice QCD (3)

- Twist rotation of these operators (at finite lattice spacing):

$$
\begin{pmatrix}
\bar{\psi}^{(d)}(\gamma_5)\psi^{(s)} \\
\bar{\psi}^{(d)}(\gamma_5)\psi^{(c)} \\
\bar{\psi}^{(d)}\psi^{(s)} \\
\bar{\psi}^{(d)}\psi^{(c)}
\end{pmatrix}
= \begin{pmatrix}
c_{l}c_{h} & s_{l}s_{h} & -i s_{l}c_{h} & + i c_{l}s_{h} \\
s_{l}s_{h} & c_{l}c_{h} & + i c_{l}s_{h} & - i s_{l}c_{h} \\
-i s_{l}c_{h} & + i c_{l}s_{h} & c_{l}c_{h} & s_{l}s_{h} \\
+ i c_{l}s_{h} & - i s_{l}c_{h} & s_{l}s_{h} & c_{l}c_{h}
\end{pmatrix}
\begin{pmatrix}
Z_{P}\bar{\chi}^{(d)}(\gamma_{5})\chi^{(s)} \\
Z_{P}\bar{\chi}^{(d)}(\gamma_{5})\chi^{(c)} \\
Z_{S}\bar{\chi}^{(d)}\chi^{(s)} \\
Z_{S}\bar{\chi}^{(d)}\chi^{(c)}
\end{pmatrix} = M_{\text{tw.rot.}}(\omega_{l},\omega_{h},Z_{P}/Z_{S})
$$

where $c_{x} = \cos(\omega_{x}/2)$ and $s_{x} = \sin(\omega_{x}/2)$ and $Z_{P}$ and $Z_{S}$ are operator dependent renormalization constants.
\[ m(K) \text{ and } m(D) \] (1)

- Starting point: correlation matrix

\[
C_{jk}(t) = \langle \Omega | O_j(t) \left(O_k(0)\right)^\dagger | \Omega \rangle
\]

\[ O_j \in \{ \overline{\chi}^{(d)} \gamma_5 \chi^{(s)} , \overline{\chi}^{(d)} \gamma_5 \chi^{(c)} , \overline{\chi}^{(d)} \chi^{(s)} , \overline{\chi}^{(d)} \chi^{(c)} \}. \]

- Three (slightly) different methods:
  
  A. Generalized eigenvalue problem.
  
  B. Fitting exponentials.
  
  C. Parity and flavor restoration.

- Most results presented in the following correspond to these two ensembles:

<table>
<thead>
<tr>
<th>\beta</th>
<th>L^3 \times T</th>
<th>\mu</th>
<th>\kappa</th>
<th>\mu_\sigma</th>
<th>\mu_\delta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.90</td>
<td>32^3 \times 64</td>
<td>0.0040</td>
<td>0.163270</td>
<td>0.150</td>
<td>0.190</td>
</tr>
<tr>
<td>1.95</td>
<td>32^3 \times 64</td>
<td>0.0035</td>
<td>0.161240</td>
<td>0.135</td>
<td>0.170</td>
</tr>
</tbody>
</table>
A. Generalized eigenvalue problem (1)

- Generalized eigenvalue problem (GEP):

\[
C_{jk}(t)v_j^{(n)}(t, t_0) = C_{jk}(t_0)v_j^{(n)}(t, t_0)\lambda^{(n)}(t, t_0).
\]

- Effective meson masses:

\[
m_{\text{effective}}^{(n)}(t, t_0) = \ln \left( \frac{\lambda^{(n)}(t, t_0)}{\lambda^{(n)}(t + a, t_0)} \right).
\]

- Fitting constants to effective mass plateaus at \( t \gg 1 \) yields meson masses.

- From the eigenvectors \( v^{(n)} \) one can read off the quantum numbers flavor and parity, i.e. \((s, -), (s, +), (c, -)\) or \((c, +)\).
A. Generalized eigenvalue problem (2)

- For $t \gg 1$ GEP yields the lowest four states in the combined $(s/c, -/+)$ sector; the $D$ is not among them.
  
  - $m(K^\pm) = 494$ MeV, $m(K^0) = 498$ MeV ($J^P = 0^-$).
  - $m(K^*_0(800)) = 672(40)$ MeV ($J^P = 0^+$).
  - $m(K^*_0(1430)) = 1425(50)$ MeV ($J^P = 0^+$).
  - $m(K(1460)) = 1400$ MeV ... 1460 MeV ($J^P = 0^-$).
  - ...
  - $m(K + \pi)$.
  - $m(K + 2 \times \pi)$.
  - ...
  - $m(D^0) = 1865$ MeV, $m(K^\pm) = 1870$ MeV ($J^P = 0^-$).
A. Generalized eigenvalue problem (3)

• Why can we still expect to get an estimate for $m(D)$ from GEP?
  – In the continuum an exact diagonalization of $C_{jk}$ is possible yielding one correlator for each of the four sectors $(s, -), (s, +), (c, -), (c, +)$
  → GEP would not yield the four lowest masses but $m(K), m(s, +), m(D)$ and $m(c, +)$.
  – At finite lattice spacing corrections are $O(a)$; at not too large temporal separations one of the four effective masses should be dominated by the $D$.

\[ \beta = 1.90, \mu = 0.0040 \]

\[ \beta = 1.95, \mu = 0.0035 \]
A. Generalized eigenvalue problem (4)

- Identification of quantum numbers \((s, -), (s, +), (c, -)\) or \((c, +)\) by rotating the eigenvectors \(v^{(n)}(t, t_0)\) to the pseudo physical basis.

\[\beta = 1.95, \mu = 0.0035\]
A. Generalized eigenvalue problem (5)

- With larger matrices (which are able to resolve all single and multi particle strange states below the \( D \)) GEP becomes exact (not feasible at currently available statistics, extremely complicated).

Marc Wagner, “The heavy-light sector of \( N_f = 2 + 1 + 1 \) twisted mass lattice QCD”, September 24, 2009
B. Fitting exponentials (1)

- Perform a $\chi^2$ minimizing fit of

$$\tilde{C}_{jk}(t) = \sum_{n=1}^{N} \left( a_j^{(n)} \right)^\dagger a_k^{(n)} \exp \left( -m^{(n)} t \right)$$

($N$ is an arbitrary number of exponentials) to the computed correlation matrix $C_{jk}(t)$, $t_{\text{min}} \leq t \leq t_{\text{max}}$.

- Similar to GEP, but less “obvious”, why it works:
  - Exponentials can end up in the same sector.
  - All exponentials will end up in the strange sectors, if large $t$ values are considered in the fit.
  - Results might depend on the initial fitting parameters.
B. Fitting exponentials (2)

- Left plot: “effective mass values” for $K$, $K^*/K + \pi$ and $D$ obtained by considering different fitting ranges $t_{\text{min}} \leq t \leq t_{\text{max}}$.

- Right plots: histograms of effective mass values for $m(K)$ and $m(D)$; the widths of these histograms are taken as the combined statistical and systematical errors for $m(K)$ and $m(D)$.

\[ \beta = 1.95, \mu = 0.0035 \]
B. Fitting exponentials (3)

- With larger matrices (which are able to resolve all single and multi particle strange states below the $D$) fitting exponentials becomes exact (not feasible at currently available statistics, extremely complicated).
C. Parity and flavor restoration (1)

- Express the correlation matrix $C_{jk}(t)$ in the physical basis in terms of the twist angles $\omega_l$ and $\omega_h$ and $Z_P/Z_S$:

$$C_{jk}^{(\text{physical})}(t; \omega_l, \omega_h, Z_P/Z_S) = M_{\text{tw.rot.}}(\omega_l, \omega_h, Z_P/Z_S)C_{jk}(t)\left(M_{\text{tw.rot.}}(\omega_l, \omega_h, Z_P/Z_S)\right)^\dagger.$$ 

- Determine $\omega_l$, $\omega_h$ and $Z_P/Z_S$ by requiring

$$C_{jk}^{(\text{physical})}(t; \omega_l, \omega_h, Z_P/Z_S)|_{j \neq k} = 0.$$

  - At finite lattice spacing and small $t$ this cannot be achieved exactly (excited states, $O(a)$ effects).
  - At large $t$ (when only the $K$ survives) it can be achieved.
  - This corresponds to removing any $K$ contribution from the diagonal correlators $C_{jj}^{(\text{physical})}$, $j \neq (s, -)$. 

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C. Parity and flavor restoration (2)

• Analyze the diagonal correlators $C_{jj}^{(\text{physical})}$ separately; one correlator for each of the four sectors $(s, -), (s, +), (c, -), (c, +)$.

• $\omega_l, \omega_h$ and $Z_P/Z_S$ are determined from parity odd/flavor non-diagonal matrix elements, which are not $O(a)$ improved.

• The “$D$ correlator” $C_{jj}^{(\text{physical})}$, $j = (c, -)$ is contaminated by $O(a)$ contributions from lighter states (not $K$, but $K^*_0$, $K + \pi$, “excited $K$”, ...) → at large $t$ the effective mass will break down to the mass value of the lightest of these states.
C. Parity and flavor restoration (3)

\[ \beta = 1.90, \mu = 0.0040 \]

A: Kaon Effective Mass

\[ \beta = 1.95, \mu = 0.0035 \]

B: Kaon Effective Mass

A: D Meson Effective Mass

B: D Meson Effective Mass

\[ \beta = 1.90, \mu = 0.0040 \]

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\[ \beta = 1.95, \mu = 0.0035 \]
Results obtained with these three methods agree within statistical errors.

Rather precise results for $m(K)$.
- Statistical error $\sim 0.2\%$.

All three methods require assumptions for $m(D)$, i.e. there is a systematical error involved.
- Way of estimating the systematical error is somewhat arbitrary.
- Combined statistical and systematical error $\lesssim 5\%$.
- Systematical error larger than statistical error.
Optimization of operators (1)

- Mesons are characterized by quantum numbers flavor and $J^P$.
- Many different meson creation operators with the same quantum numbers.
  - Width of the operator and the corresponding trial state.
    * Smearing method and parameters (we use Gaussian smearing).
    * Ground state overlaps are significantly larger.
    * Optimized smearing essential for $m(D)$.

\[ \beta = 1.9, \ L \times T = 24^3 \times 48, \ \mu = 0.0100, \ \kappa = 0.163255, \ \mu_\sigma = 0.15, \ \mu_\delta = 0.19 \]
Inclusion of $\gamma_0$, i.e. operators

$$O_j \in \left\{ \bar{\chi}^{(d)} \gamma_0 \gamma_5 \chi^{(s)}, \bar{\chi}^{(d)} \gamma_0 \gamma_5 \chi^{(c)}, \bar{\chi}^{(d)} \gamma_0 \chi^{(s)}, \bar{\chi}^{(d)} \gamma_0 \chi^{(c)} \right\}.$$  

* Ground state overlaps are slightly smaller.

...
Decay constants $f_K$ and $f_D$

- Decay constants $f_K$ and $f_D$ can be obtained via

\[
\begin{align*}
  f_K &= \frac{\mu + \mu_\sigma - (Z_P/Z_S)\mu_\delta}{m(K)^{3/2}} \langle \Omega \mid \frac{1}{\sqrt{2}} \left( P^K + P^D - i\frac{Z_S}{Z_P} (S^K - S^D) \right) \mid K \rangle \\
  f_D &= \frac{\mu + \mu_\sigma + (Z_P/Z_S)\mu_\delta}{m(D)^{3/2}} \langle \Omega \mid \frac{1}{\sqrt{2}} \left( P^K + P^D + i\frac{Z_S}{Z_P} (S^K - S^D) \right) \mid D \rangle \\
  P^{K/D} &= \left( \bar{\chi}^{(d)} \gamma_5 \chi^{(s/c)} \right)^\dagger, \quad S^{K/D} &= \left( \bar{\chi}^{(d)} \chi^{(s/c)} \right)^\dagger,
\end{align*}
\]

where $\langle K \mid K \rangle = 1$ and $\langle D \mid D \rangle = 1$.

- $Z_P/Z_S$ is determined from parity odd/flavor non-diagonal matrix elements, which are not $O(a)$ improved (cf. method C.).

- For $f_D$ similar problems as for $m(D)$. 

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Vector mesons $K^*$ and $D^*$ (1)

- Vector mesons ($J^P = 1^-$):
  
  \[ m(K^*(892)) = 892 \text{ MeV}. \]
  \[ m(D^*(2007)^0) = 2007 \text{ MeV}, \quad m(D^*(2010)^\pm) = 2010 \text{ MeV}. \]

- Meson creation operators:

\[ \mathcal{O}_j \in \left\{ \bar{\chi}^{(d)}(d) \gamma_j \chi^{(s)}, \quad \bar{\chi}^{(d)}(d) \gamma_j \chi^{(c)}, \quad \bar{\chi}^{(d)}(d) \gamma_j \gamma_5 \chi^{(s)}, \quad \bar{\chi}^{(d)}(d) \gamma_j \gamma_5 \chi^{(c)} \right\}. \]
Vector mesons $K^*$ and $D^*$ (2)

- Preliminary results ($\beta = 1.9$, $L^3 \times T = 24^3 \times 48$, $\kappa = 0.163270$, $\mu = 0.0040$, $\mu_\sigma = 0.15$, $\mu_\delta = 0.19$):
  
  - $m(K^*)/m(K) = 1.77(5)$ (PDG: $m(K^*)/m(K) \approx 1.80$).
  
  - $m(D^*)/m(D) = 1.08(4)$ (PDG: $m(D^*)/m(D) \approx 1.08$).

- $K^*$ problematic, because it is a resonance: $K^*$ can decay to $K + \pi$. 

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Status at “Lattice 2009”

$(2m(K)^2 - m_{PS}^2)r_0^2$ as a function of $(m_{PS}r_0)^2$

$(m(K)/m(K^*))^2$ as a function of $(m_{PS}r_0)^2$

$m(D)r_0$ as a function of $(m_{PS}r_0)^2$
Mixed action OS setup (1)

- Heavy Dirac operator in the valence sector:

\[
Q(\chi^{(h),\text{valence}}) = \gamma_\mu D_\mu + m + i\gamma_5 \begin{pmatrix} +\mu_1 & 0 \\ 0 & -\mu_2 \end{pmatrix} - \frac{a}{2}\Box.
\]

- Both heavy and light flavors are diagonal
  → two distinct sectors \((s, -/+\)) and \((c, -/+\)) instead of four
  → only “problems” with parity
  → determination of \(m(D)\) becomes easy (the \(D\) is the lightest state in the charm sector).

- Formulation cannot be used during simulations (sign problem).
Mixed action OS setup (2)

• Matching of valence and sea quark masses:
  
  – Method 1:
    \[ \mu_{1,2} = \mu_\sigma \mp \frac{Z_P}{Z_S} \mu_\delta \]
    
    \( Z_P/Z_S \) has not been determined in a satisfactory way yet).
  
  – Method 2:
    tune \( \mu_1 \) and \( \mu_2 \) such that \( m(K) \) and \( m(D) \) are the same both in the unitary and in the mixed action setup (what we do at the moment).
Conclusions

• Unitary setup:
  – Precise results in the strange sector ($m(K)$, ...).
  – Problems in the charm sector ($m(D)$, ...), due to twisted mass flavor breaking.

• Mixed action OS setup:
  – A promising method to do charm physics.
  – Unitary setup (at the moment) necessary, to achieve a matching of quark masses.