PROCEEDINGS OF SCIENCE

SFB/CPP-10-80, DESY 10-127, HU-EP-10/48

arXiv:1009.2074v1 [hep-lat] 10 Sep 2010

Kaon and D meson masses with $N_f = 2+1+1$ twisted mass lattice QCD

ETM Collaboration: Rémi Baron[a], Philippe Boucaud[b], Jaume Carbonell[c], Vincent Drach[c], Federico Farchioni[d], Gregorio Herdoiza[e], Karl Jansen[e], Chris Michael[f], István Montvay[g], Elisabetta Pallante[h], Siebren Reker[h], Carsten Urbach[i], Marc Wagner*[j], Urs Wenger[k]

[a] CEA, Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France
[b] Laboratoire de Physique Théorique (Bât. 210), CNRS et Université Paris-Sud XI, Centre d'Orsay, 91405 Orsay-Cedex, France
[c] Laboratoire de Physique Subatomique et Cosmologie, 53 avenue des Martyrs, 38026 Grenoble, France
[d] Universität Münster, Institut für Theoretische Physik, Wilhelm-Klemm-Straße 9, D-48149 Münster, Germany
[e] NIC, DESY, Platanenallee 6, D-15738 Zeuthen, Germany
[f] Division of Theoretical Physics, University of Liverpool, L69 3BX Liverpool, United Kingdom
[g] Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22603 Hamburg, Germany
[h] Centre for Theoretical Physics, University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands
[i] Helmholtz-Institut für Strahlen- und Kernphysik (Theorie) and Bethe Center for Theoretical Physics, Universität Bonn, 53115 Bonn, Germany
[j] Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin, Germany
[k] Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstr. 5, CH-3012 Bern, Switzerland

We discuss the computation of the kaon and D meson masses in the $N_f = 2+1+1$ twisted mass lattice QCD setup, where explicit heavy flavor and parity breaking occurs at finite lattice spacing. We present three methods suitable in this context and verify their consistency.

The XXVIII International Symposium on Lattice Field Theory, Lattice2010
June 14-19, 2010
Villasimius, Italy

*Speaker.

© Copyright owned by the author(s) under the terms of the Creative Commons Attribution-NonCommercial-ShareAlike Licence.

1. Introduction

The European Twisted Mass Collaboration (ETMC) is currently performing large scale simulations with $N_f = 2+1+1$ flavors of dynamical quarks using Wilson twisted mass lattice QCD [1, 2, 3].

Particular problems are caused by the non-degenerate strange/charm quark doublet, since besides the usual twisted mass parity breaking the strange and charm quark numbers are not conserved. The latter amounts to contamination of correlation functions by intermediate states with wrong flavor quantum numbers. In particular, correlation functions of charmed mesons and baryons obtain small contributions from similar strange systems, which are significantly lighter and, therefore, inevitably dominate at large temporal separations. In this paper we discuss these problems in the context of the kaon and D meson masses, which are important quantities already at the stage of generating gauge field configurations, when tuning the strange and charm quark masses to their physical values. We present three methods to overcome these problems and demonstrate their consistency. This work is a summary of a more detailed recent paper [4].

2. Simulation setup

The gauge action is the Iwasaki action [5]. The fermion action is Wilson twisted mass,

$$S_{\mathrm{F,light}}[\chi^{(l)},\bar{\chi}^{(l)},U] = a^4\sum_x \bar{\chi}^{(l)}(x)\Big(D_{\mathrm{W}}(m_0)+i\mu\gamma_5\tau_3\Big)\chi^{(l)}(x) \tag{2.1}$$

$$S_{\mathrm{F,heavy}}[\chi^{(h)},\bar{\chi}^{(h)},U] = a^4\sum_x \bar{\chi}^{(h)}(x)\Big(D_{\mathrm{W}}(m_0)+i\mu_\sigma\gamma_5\tau_1+\tau_3\mu_\delta\Big)\chi^{(h)}(x) \tag{2.2}$$

for the light degenerate up/down doublet [6] and the heavy non-degenerate strange/charm doublet [7] respectively, where D_{W} denotes the standard Wilson Dirac operator. $\kappa = 1/(2m_0+8)$ is tuned to maximal twist by requiring $m^{\mathrm{PCAC}}_{\chi^{(l)}} = 0$, which guarantees automatic $\mathcal{O}(a)$ improvement for physical quantities, e.g. the here considered kaon and D meson masses. We also refer to [8], where this $N_f = 2+1+1$ twisted mass setup has been pioneered.

All results presented in the following correspond to computations on 1042 gauge field configurations from ensemble B35.32 [3] characterized by gauge coupling $\beta = 1.95$, lattice extension $L^3\times T = 32^3\times 64$ and bare untwisted and twisted quark masses $\kappa = 0.161240$, $\mu = 0.0035$, $\mu_\sigma = 0.135$ and $\mu_\delta = 0.170$. The corresponding lattice spacing is $a \approx 0.078\,\mathrm{fm}$, the pion mass $m_{\mathrm{PS}} \approx 318\,\mathrm{MeV}$.

3. Quantum numbers, physical and twisted basis meson creation operators

In Wilson twisted mass lattice QCD parity is not a symmetry and the heavy flavors cannot be diagonalized – both symmetries are broken at $\mathcal{O}(a)$. Consequently, instead of the four QCD heavy-light meson sectors labeled by heavy flavor and parity, $(s,-)$, $(s,+)$, $(c,-)$ and $(c,+)$, there is only a single combined heavy-light meson sector $(s/c,-/+)$ in twisted mass lattice QCD. In contrast to QCD, where the D meson is the lightest state in the $(c,-)$ sector, it is a highly excited state in the combined $(s/c,-/+)$ sector of twisted mass lattice QCD. This in turn causes severe problems for

the computation of m_D, since the determination of excited states is inherently difficult, when using lattice methods.

To create kaons and D mesons a suitable set of operators is

$$\mathcal{O}_j \;\in\; \Big\{ +i\bar{\chi}^{(d)}\gamma_5\chi^{(s)}\,,\, -i\bar{\chi}^{(d)}\gamma_5\chi^{(c)}\,,\, +\bar{\chi}^{(d)}\chi^{(s)}\,,\, -\bar{\chi}^{(d)}\chi^{(c)} \Big\}. \tag{3.1}$$

In the continuum the twisted basis quark fields χ and their physical basis counterparts ψ are related by the twist rotation

$$\begin{pmatrix} \psi^{(u)} \\ \psi^{(d)} \end{pmatrix} \;=\; \exp\Big(i\gamma_5\tau_3\omega_l/2\Big) \begin{pmatrix} \chi^{(u)} \\ \chi^{(d)} \end{pmatrix} \quad , \quad \begin{pmatrix} \psi^{(s)} \\ \psi^{(c)} \end{pmatrix} \;=\; \exp\Big(i\gamma_5\tau_1\omega_h/2\Big) \begin{pmatrix} \chi^{(s)} \\ \chi^{(c)} \end{pmatrix}. \tag{3.2}$$

ω_l and ω_h denote the light and heavy twist angles, which are $\pi/2$ at maximal twist. At finite lattice spacing the procedure is more complicated, since renormalization factors have to be included. The heavy-light meson creation operators (3.1) and the corresponding renormalized operators in the physical basis transform into each other via

$$\begin{pmatrix} +i\bar{\psi}^{(d)}\gamma_5\psi^{(s)} \\ -i\bar{\psi}^{(d)}\gamma_5\psi^{(c)} \\ +\bar{\psi}^{(d)}\psi^{(s)} \\ -\bar{\psi}^{(d)}\psi^{(c)} \end{pmatrix}^R \;=\; \underbrace{\begin{pmatrix} +c_lc_h & -s_ls_h & -s_lc_h & -c_ls_h \\ -s_ls_h & +c_lc_h & -c_ls_h & -s_lc_h \\ +s_lc_h & +c_ls_h & +c_lc_h & -s_ls_h \\ +c_ls_h & +s_lc_h & -s_ls_h & +c_lc_h \end{pmatrix}}_{=\mathcal{M}(\omega_l,\omega_h)} \begin{pmatrix} +iZ_P\bar{\chi}^{(d)}\gamma_5\chi^{(s)} \\ -iZ_P\bar{\chi}^{(d)}\gamma_5\chi^{(c)} \\ +Z_S\bar{\chi}^{(d)}\chi^{(s)} \\ -Z_S\bar{\chi}^{(d)}\chi^{(c)} \end{pmatrix}, \tag{3.3}$$

where $c_x = \cos(\omega_x/2)$, $s_x = \sin(\omega_x/2)$ and Z_P and Z_S are operator dependent renormalization constants.

The starting point for the three analysis methods presented in the following sections 4 to 6 are the 4×4 correlation matrices

$$C_{jk}(t) \;=\; \langle\Omega|\mathcal{O}_j(t)\Big(\mathcal{O}_k(0)\Big)^\dagger|\Omega\rangle \tag{3.4}$$

of spatially extended, i.e. APE and Gaussian smeared versions of twisted basis heavy-light meson creation operators (3.1). The smearing parameters have been optimized by minimizing effective masses at small temporal separations (cf. [4] for details).

4. Method 1: solving a generalized eigenvalue problem

One possibility to determine m_K and m_D is to solve the generalized eigenvalue problem

$$C_{jk}(t)v_j^{(n)}(t,t_0) \;=\; C_{jk}(t_0)\lambda^{(n)}(t,t_0)v_j^{(n)}(t,t_0)\,, \tag{4.1}$$

cf. e.g. [9] and references therein. From the eigenvalues $\lambda^{(n)}$ one then computes four effective masses $m^{(n)}_{\text{effective}}$ by solving

$$\frac{\lambda^{(n)}(t,t_0)}{\lambda^{(n)}(t+1,t_0)} \;=\; \frac{\exp(-m^{(n)}_{\text{effective}}(t,t_0)t) + \exp(-m^{(n)}_{\text{effective}}(t,t_0)(T-t))}{\exp(-m^{(n)}_{\text{effective}}(t,t_0)(t+1)) + \exp(-m^{(n)}_{\text{effective}}(t,t_0)(T-(t+1)))}, \tag{4.2}$$

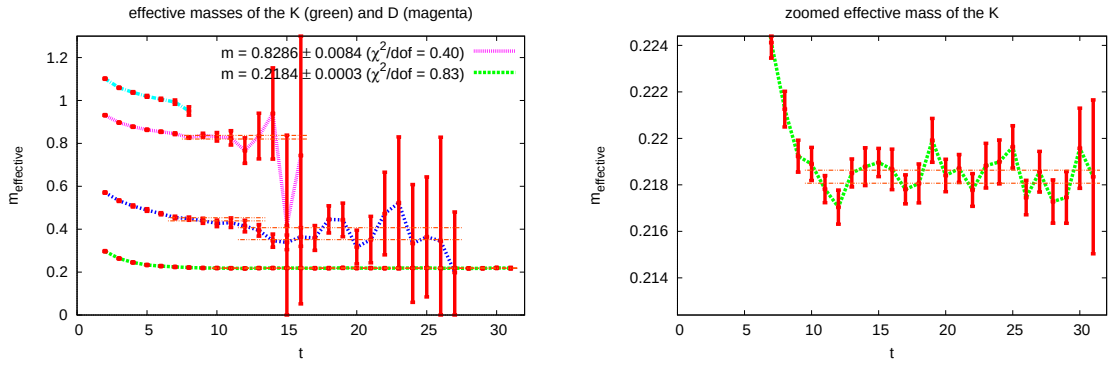

Figure 1: left: effective masses obtained from the 4×4 correlation matrix (3.4) by solving the generalized eigenvalue problem (4.1) and (4.2) and corresponding plateau fits; right: zoomed effective mass of the lowest state, which has been identified as the kaon.

where T is the temporal extension of the lattice and the exponentials $e(-m^{(n)}_{\text{effective}}(t,t_0)(T-t))$ and $e(-m^{(n)}_{\text{effective}}(t,t_0)(T-(t+1)))$ take care of effects due to the temporal periodicity of the lattice. Heavy-light meson masses are finally determined by fitting constants to effective mass plateaus at temporal separations $t \gg 1$. Results are shown in Figure 1.

It is well known that for sufficiently large temporal separations t the generalized eigenvalue problem (4.1) and (4.2) yields the lowest states in the sector considered, i.e. in our case the four lowest states in the combined $(s/c,-/+)$ sector. The D meson ($m(D) \approx 1868\,\text{MeV}$), however, is not among them. Lighter states include

- the kaon and its radial excitations,
  $m(K) \approx 496\,\text{MeV}$, $m(K(1460)) = 1400\,\text{MeV} - 1460\,\text{MeV}$, ...
- parity partners of the kaon
  $m(K_0^*(800)) = 672(40)\,\text{MeV}$, $m(K_0^*(1430)) = 1425(50)\,\text{MeV}$, ...
- multi particle states
  $m(K+\pi)$, $m(K+2\times\pi)$, ...

At first glance it seems that the 4×4 correlation matrix (3.4) is not sufficient to determine m_D, but that one needs a significantly larger correlation matrix, which is able to resolve all states below the D meson. Note, however, that in the continuum an exact diagonalization of C_{jk} is possible yielding one correlator for each of the four sectors $(s,-)$, $(s,+)$, $(c,-)$, $(c,+)$. Hence the generalized eigenvalue problem would not yield the four lowest masses of the $(s/c,-/+)$ sector, but m_K, $m_{(s,+)}$, m_D and $m_{(c,+)}$. At finite lattice spacings such a diagonalization is, of course, only approximately possible. However, discretization artefacts, which are responsible for that, only appear at $\mathcal{O}(a)$ and are thus expected to be small. Therefore, at not too large temporal separations one of the four effective masses should be dominated by the D meson and, consequently, provide an estimate for m_D.

One can check that this is indeed the case by twist rotating the eigenvectors $\mathbf{v}^{(n)}$ to the pseudo physical basis, which is defined by (3.3) with $Z_P = Z_S = 1$. Then one can read off the approximate

flavor and parity content of each of the four states corresponding to the four effective mass plateaus. As shown in Figure 2, the lowest state is dominated by the physical basis operator $\bar{\psi}^{(d)}\gamma_5\psi^{(s)}$ and, therefore, interpreted as the kaon, while the second excited state is dominated by $\bar{\psi}^{(d)}\gamma_5\psi^{(c)}$, i.e. corresponds to the D meson.

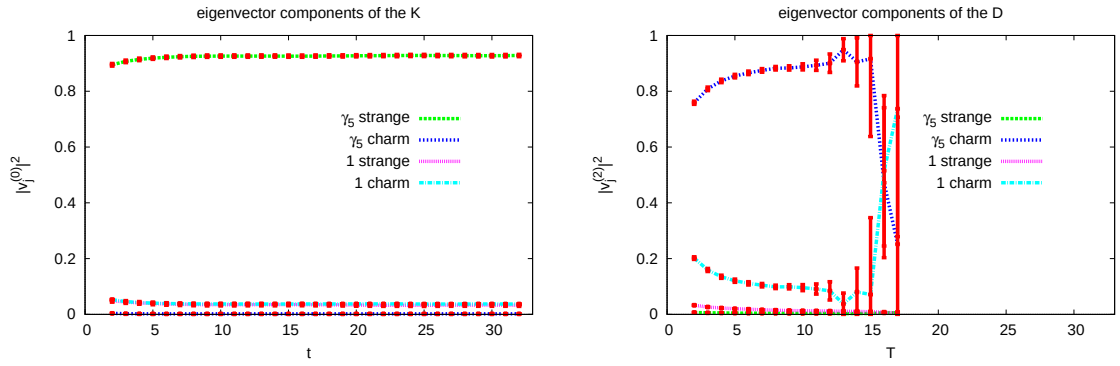

Figure 2: left: squared pseudo physical basis eigenvector components of the lowest state $|v_j^{(0)}|^2$, which is interpreted as the kaon; right: squared pseudo physical basis eigenvector components of the second excited state $|v_j^{(2)}|^2$, which is interpreted as the D meson.

5. Method 2: fitting exponentials

An alternative approach to determine m_K and m_D is to perform a χ^2 minimizing fit of

$$\sum_{n=1}^{N} (a_j^{(n)})^\dagger a_k^{(n)} \Big(\exp\Big(-m_n t\Big) + \exp\Big(-m_n(T-t)\Big)\Big), \tag{5.1}$$

i.e. of N exponentials to the computed correlation matrix C_{jk} in a suitably chosen window of temporal separations t. Notice that T is the temporal extension of the lattice and the second exponential $\exp(-m_n(T-t))$ takes care of effects due to the lattice temporal periodicity. The masses m_n can be interpreted by analyzing the prefactors $a_j^{(n)}$, which is very similar to what has been explained in more detail in the previous section for the eigenvector components provided by the generalized eigenvalue problem.

As before we find that the lowest state is a kaon, while the second excited state is dominated by the physical basis operator $\bar{\psi}^{(d)}\gamma_5\psi^{(c)}$ and, hence, should correspond to the D meson.

6. Method 3: heavy flavor/parity restoration

Our third approach is based on the twist rotation of heavy-light meson creation operators (3.3). In a first step we express the correlation matrix C_{jk} in the physical basis in terms of the twist angles ω_l and ω_h and the ratio of renormalization factors Z_P and Z_S:

$$\begin{aligned} C^{\text{physical},R}(t;\omega_l,\omega_h,Z_P/Z_S) &= \\ &= \mathscr{M}(\omega_l,\omega_h)\,\text{diag}(Z_P,Z_P,Z_S,Z_S)\,C(t)\,\text{diag}(Z_P,Z_P,Z_S,Z_S)\,\mathscr{M}^\dagger(\omega_l,\omega_h), \end{aligned} \tag{6.1}$$

where the matrix $\mathscr{M}$ has been defined in (3.3). We then determine ω_l, ω_h and Z_P/Z_S by requiring

$$C_{jk}^{\text{physical},R}(t;\omega_l,\omega_h,Z_P/Z_S)\Big|_{j\neq k} \;=\; 0. \tag{6.2}$$

At finite lattice spacing and small temporal separations t this cannot be achieved exactly, because of $\mathscr{O}(a)$ heavy flavor and parity breaking effects and the presence of excited states. However, at sufficiently large t, where only the kaon survives, the condition (6.2) can be realized. It amounts to removing any kaon contribution from the diagonal correlators $C_{jj}^{\text{physical},R}$, $j \neq (s,-)$.

Finally we analyze the diagonal correlators $C_{jj}^{\text{physical},R}$ individually. There is one correlator for each of the four sectors $(s,-)$, $(s,+)$, $(c,-)$ and $(c,+)$. The effective mass plateaus corresponding to the $(s,-)$ and the $(c,-)$ diagonal correlator yield the heavy-light meson masses m_K and m_D, respectively.

7. Conclusions and outlook

Results for m_K and m_D obtained with our three methods agree within statistical and systematic errors, see Table 1 and Figure 3. For a detailed discussion, of how statistical and systematic errors have been determined, we refer to [4]. We are able to determine m_K in a rigorous way with rather high statistical precision (statistical error $\lesssim$0.4%). On the other hand all three methods require assumptions, when computing m_D, which amount to a systematical error being involved. Nevertheless, the combined statistical and systematical error for m_D is $\lesssim$2.5%.

	method 1	method 2	method 3
m_K	0.2184(3)	0.2177(8)	0.2184(3)
m_D	0.829(8)	0.835(20)	0.823(15)

Table 1: comparison of kaon and D meson masses determined with the three methods presented.

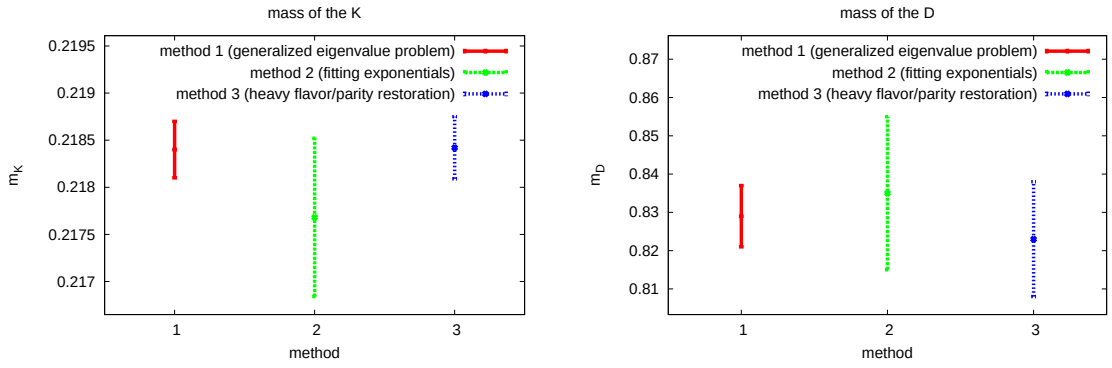

Figure 3: comparison of kaon and D meson masses determined with the three methods presented.

Being able to determine m_K and m_D is very important for tuning the strange and charm quark masses to their physical values. For precision charm physics, however, we intend to use a mixed

action Osterwalder-Seiler setup [10]. First steps in this direction are currently under way and have been reported during this conference [11].

Acknowledgments

The computer time for this project was made available to us by the John von Neumann-Institute for Computing (NIC) on the JUMP, Juropa and Jugene systems in Jülich and apeNEXT system in Zeuthen, BG/P and BG/L in Groningen, by BSC on Mare-Nostrum in Barcelona (`www.bsc.es`) and by the computer resources made available by CNRS on the BlueGene system at GENCI-IDRIS Grant 2009-052271 and CCIN2P3 in Lyon. We thank these computer centers and their staff for all technical advice and help.

This work has been supported in part by the DFG Sonderforschungsbereich TR9 Computergestützte Theoretische Teilchenphysik and the EU Integrated Infrastructure Initiative Hadron Physics (I3HP) under contract RII3-CT-2004-506078. We also thank the DEISA Consortium (co-funded by the EU, FP6 project 508830) for support within the DEISA Extreme Computing Initiative (`www.deisa.org`).

References

[1] R. Baron *et al.* [ETM Collaboration], PoS **LATTICE2008**, 094 (2008) [arXiv:0810.3807 [hep-lat]].

[2] R. Baron *et al.*, PoS **LATTICE2009**, 104 (2009) [arXiv:0911.5244 [hep-lat]].

[3] R. Baron *et al.* [ETM Collaboration], JHEP **1006**, 111 (2010) [arXiv:1004.5284 [hep-lat]].

[4] R. Baron *et al.* [ETM Collaboration], arXiv:1005.2042 [hep-lat].

[5] Y. Iwasaki, Nucl. Phys. B **258**, 141 (1985).

[6] **ALPHA** Collaboration, R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz, JHEP **0108**, 058 (2001) [arXiv:hep-lat/0101001].

[7] R. Frezzotti and G. C. Rossi, Nucl. Phys. Proc. Suppl. **128** (2004) 193 [arXiv:hep-lat/0311008].

[8] T. Chiarappa *et al.*, Eur. Phys. J. C **50**, 373 (2007) [arXiv:hep-lat/0606011].

[9] B. Blossier, M. Della Morte, G. von Hippel, T. Mendes and R. Sommer, JHEP **0904**, 094 (2009) [arXiv:0902.1265 [hep-lat]].

[10] R. Frezzotti and G. C. Rossi, JHEP **0410** (2004) 070 [arXiv:hep-lat/0407002].

[11] C. Urbach *et al.* [ETM Collaboration], talk by C. Urbach at "XXVIIIth International Symposium on Lattice Field Theory", Villasimius, Sardinia (2010).