Towards leading isospin breaking effects in mesonic masses on open boundaries

Andreas Risch[1]
andreas.risch@uni-mainz.de

Hartmut Wittig [1,2]
hartmut.wittig@uni-mainz.de

[1]PRISMA Cluster of Excellence and Institut für Kernphysik, University of Mainz, Germany

[2]Helmholtz Institute Mainz, University of Mainz, Germany

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Motivation

- Lattice QCD simulations are usually performed with an isosymmetric setup:
  - degenerate light quark masses
  - neutral quarks
- However: Isospin is not an exact symmetry! [Patrignani et al., 2016]

	u	d	π^+	π^0	K^+	K^0
m [MeV]	$2.2^{+0.5}_{-0.4}$	$4.7^{+0.5}_{-0.3}$	139.57	134.97	493.67	497.61
q [e]	$\frac{2}{3}$	$-\frac{1}{3}$	1	0	1	0

$\Rightarrow$ Neglecting isospin breaking effects can lead to systematic errors depending on the investigated observable

- Strong isospin breaking and QED effects may come in with opposite signs
- Include light quark mass splitting and QED in lattice simulations

Isospin breaking effects on CLS open boundary ensembles

Approaches investigating isospin breaking effects:

- Generation of combined QCD+QED gauge configurations [Campos et al., 2018]
- Combine existing QCD gauge configurations with new QED gauge configurations [Borsanyi et al., 2015]
- Expand QCD+QED perturbatively around $\mathrm{QCD_{iso}}$ [de Divitiis et al., 2012, de Divitiis et al., 2013]

Our work:

- Use Coordinated Lattice Simulations (CLS) N_f=2+1 QCD ensembles with open boundaries (reduces topology freezing)
- Use non-compact lattice QED:
  $\Rightarrow$ Formulation for open boundaries required
- Naive non-compact lattice QED suffers from zero-mode divergences:
  $\Rightarrow$ Use $\mathrm{QED_L}$ as an IR regularised theory, i.e. $A^{p\mu} = 0$ for $\vec{p} = 0$
  [Hayakawa and Uno, 2008, Borsanyi et al., 2015, Patella, 2017]
- Introduce hadronic renormalisation scheme adapted to QCD+QED

QED_L on open boundaries

- Open boundary gauge action on the lattice $\prod_{\mu=0}^{3}\{0,\dots,X^\mu-1\}$ (cf. [Lüscher and Schaefer, 2011] for compact action):

$$S_{\gamma,0}[F] = \frac{1}{4}\sum_{x^0=0}^{X^0-2}\sum_{\vec{x}}\sum_{\mu=1}^{3}\left(F^{x0\mu}F^{x0\mu} + F^{x\mu0}F^{x\mu0}\right) + \frac{1}{4}\sum_{x^0=0}^{X^0-1}\sum_{\vec{x}}\sum_{\substack{\mu,\nu=1\\ \mu\neq\nu}}^{3} F^{x\mu\nu}F^{x\mu\nu}$$

$\Rightarrow$ Implicit boundary condition (electric field vanishes at temporal boundaries):

$$F^{x0\mu}|_{x^0=-1,X^0-1} = F^{x\mu0}|_{x^0=-1,X^0-1} = 0 \quad \mu=1,2,3$$

- Implement boundary conditions for F by homogeneous boundary conditions on A:

$$F^{x\mu\nu} = -F^{x\nu\mu} = (\partial^{\mathrm{f}\mu}A^\nu)^x - (\partial^{\mathrm{f}\nu}A^\mu)^x \qquad (\partial^{\mathrm{f}\mu}A^\nu)^x = A^{x+\hat{\mu},\nu} - A^{x\nu}$$

$$\text{Dirichlet}: \quad A^{x0}|_{x^0=-1,X^0-1} = 0 \quad \text{Neumann}: \quad (\partial^{\mathrm{f}0}A^\mu)^x|_{x^0=-1,X^0-1} = 0 \quad \mu=1,2,3$$

$\Rightarrow$ partial gauge fixing (appropriate gauge transformation exists!)

- Boundary conditions imply redefinition of lattice derivatives

QED$_\mathrm{L}$ on open boundaries

- Make use of photon action with photon operator Δ in generalised Coulomb gauge:

$$S_\gamma[A] = \frac{1}{2} A \Delta A$$

- Define transformations to block-diagonalise Δ:
  Sine (for Dirichlet), Cosine (for Neumann) and Fourier (for periodic)
- Block-diagonal photon propagator Σ in Coulomb gauge:

$$\Sigma^{p}{}_{p} = \frac{1}{(\sum_{\sigma=1}^{3} p_\mathrm{P}^{\mathrm{f}\sigma} p_\mathrm{P}^{\mathrm{b}\sigma})(p_\mathrm{N}^{\mathrm{f}0} p_\mathrm{D}^{\mathrm{b}0} + \sum_{\sigma=1}^{3} p_\mathrm{P}^{\mathrm{f}\sigma} p_\mathrm{P}^{\mathrm{b}\sigma})} \cdot \left(\begin{pmatrix} p_\mathrm{N}^{\mathrm{f}0} p_\mathrm{D}^{\mathrm{b}0} & 0 & 0 & 0 \\ 0 & -p_\mathrm{P}^{\mathrm{f}1} p_\mathrm{P}^{\mathrm{b}1} & -p_\mathrm{P}^{\mathrm{f}1} p_\mathrm{P}^{\mathrm{b}2} & -p_\mathrm{P}^{\mathrm{f}1} p_\mathrm{P}^{\mathrm{b}3} \\ 0 & -p_\mathrm{P}^{\mathrm{f}2} p_\mathrm{P}^{\mathrm{b}1} & -p_\mathrm{P}^{\mathrm{f}2} p_\mathrm{P}^{\mathrm{b}2} & -p_\mathrm{P}^{\mathrm{f}2} p_\mathrm{P}^{\mathrm{b}3} \\ 0 & -p_\mathrm{P}^{\mathrm{f}3} p_\mathrm{P}^{\mathrm{b}1} & -p_\mathrm{P}^{\mathrm{f}3} p_\mathrm{P}^{\mathrm{b}2} & -p_\mathrm{P}^{\mathrm{f}3} p_\mathrm{P}^{\mathrm{b}3} \end{pmatrix} + (\sum_{\sigma=1}^{3} p_\mathrm{P}^{\mathrm{f}\sigma} p_\mathrm{P}^{\mathrm{b}\sigma}) \cdot \mathbb{1} \right)$$

- Lattice momenta depend on boundary conditions:

$$p_\mathrm{D}^{\mathrm{b}0} = 2\mathrm{i}\sin(p^0/2) \qquad p_\mathrm{N}^{\mathrm{f}0} = -2\mathrm{i}\sin(p^0/2) \qquad p^0 \in \frac{\pi}{X^0}\{(0,)1,\ldots,X^0-1\}$$

$$p_\mathrm{P}^{\mathrm{b}\mu} = -\mathrm{i}(1-\exp(-\mathrm{i}p^\mu)) \qquad p_\mathrm{P}^{\mathrm{f}\mu} = -\mathrm{i}(\exp(\mathrm{i}p^\mu)-1) \qquad p^\mu \in \frac{2\pi}{X^\mu}\{0,\ldots,X^\mu-1\}$$

- Zero-mode elimination in QED$_\mathrm{L}$:

$$\Sigma^{p\mu}{}_{p\nu} = 0 \text{ for } \vec{p} = 0, \forall \mu, \nu$$

Isospin breaking by reweighting on QCD_{iso}

- Consider the space of QCD+QED like theories paramerised by $\varepsilon = (m_{\text{u}}, m_{\text{d}}, m_{\text{s}}, \beta, e^2)$:

$$S[U,A,\Psi,\overline{\Psi}] = S_{\text{g}}[U] + S_\gamma[A] + S_{\text{q}}[U,A,\Psi,\overline{\Psi}]$$
$$S_{\text{q}}[U,A,\Psi,\overline{\Psi}] = \overline{\Psi} D[U,A]\Psi$$

- QCD_{iso} is contained in this space with $\varepsilon^{(0)} = (m_{\text{u}}^{(0)}, m_{\text{d}}^{(0)}, m_{\text{s}}^{(0)}, \beta^{(0)}, 0)$ and $m_{\text{u}}^{(0)} = m_{\text{d}}^{(0)}$:

$$\langle O[U]\rangle_{\text{eff}}^{(0)} = \frac{1}{Z^{(0)}} \int DU \exp\left(-S_{\text{g}}^{(0)}[U]\right) Z_{\text{q}}^{(0)}[U]\, O[U]$$

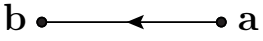
- QCD+QED can be related to QCD_{iso} by reweighting:

$$\left\langle O[U,A,\Psi,\overline{\Psi}]\right\rangle = \frac{\left\langle R[U] \left\langle O[U,A,\Psi,\overline{\Psi}]\right\rangle_{\text{q}\gamma}\right\rangle_{\text{eff}}^{(0)}}{\langle R[U]\rangle_{\text{eff}}^{(0)}}$$
$$R[U] = \frac{\exp(-S_{\text{g}}[U]) Z_{\text{q}\gamma}[U]}{\exp(-S_{\text{g}}^{(0)}[U]) Z_{\text{q}}^{(0)}[U]}$$

- Evaluate $\left\langle O[U,A,\Psi,\overline{\Psi}]\right\rangle_{\text{q}\gamma}$ and $R[U]$ as by a perturbative expansion in $\Delta\varepsilon = \varepsilon - \varepsilon^{(0)}$ around $\varepsilon^{(0)}$ [de Divitiis et al., 2012, de Divitiis et al., 2013]

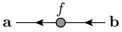
Perturbative treatment of isospin breaking effects

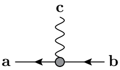
- Isosymmetric quark propagator ($\mathbf{a},\mathbf{b} \equiv (xfcs)$) and photon propagator ($\mathbf{c} \equiv (x\mu)$):

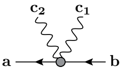
$S^{(0)}[U]^{\mathbf{b}}{}_{\mathbf{a}} =$ 

$\Sigma^{\mathbf{c_2}}{}_{\mathbf{c_1}} =$ 

- Expansion of Dirac operator in terms of $\Delta m_f = m_f - m_f^{(0)}$ with $f \in \{\mathrm{u},\mathrm{d},\mathrm{s}\}$ and e:

$D[U,A]^{\mathbf{a}}{}_{\mathbf{b}} = D^{(0)}[U]^{\mathbf{a}}{}_{\mathbf{b}} - \sum_f \Delta m_f$ 

$- e$ 

$A^{\mathbf{c}} - \frac{1}{2}e^2$ 

$A^{\mathbf{c_2}} A^{\mathbf{c_1}} + O(e^3)$

- Expansion in terms of $\Delta\beta = \beta - \beta^{(0)}$:

$\frac{\exp(-S_{\mathrm{g}}[U])}{\exp(-S_{\mathrm{g}}^{(0)}[U])} = 1 + \Delta\beta$ 

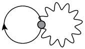
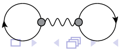
$+ O(\Delta\beta^2)$

$= -\frac{1}{\beta^{(0)}} S_{\mathrm{g}}^{(0)}[U]$

- Expansion of $R[U]$:

$R[U] = Z_\gamma^{(0)} \Big(1 + \sum_f \Delta m_f$ 

$+ \Delta\beta$ 

$+ e^2$  $+ e^2$  $+ e^2$  $+ O(\Delta\varepsilon^2) \Big)$

Analysis setup

- Electromagnetic coupling does not renormalise for first order isospin breaking effects:

$$e^2 = 4\pi\alpha$$

- Fix parameters Δm_u, Δm_d, Δm_s by hadronic renormalisation scheme:

$$\frac{1}{2}(m_{\pi^+} + m_{\pi^0}) \qquad \frac{1}{2}(m_{K^+} + m_{K^0}) \qquad m_{K^+} - m_{K^0}$$

- Scale setting (scheme not chosen yet):

$$a = a^{(0)} + \sum_l \Delta\varepsilon_l a_l^{(1)} + O(\Delta\varepsilon^2)$$

Tune $\Delta\beta$ such that scale is unchanged between QCD+QED and $\mathrm{QCD_{iso}}$:

$$\sum_l \Delta\varepsilon_l a_l^{(1)} = 0$$

$\Rightarrow$ $\Delta\beta$ depends on other expansion parameters

Mass extraction from 2-point functions

- Asymptotic behaviour of mesonic 2-point correlation function:

$$C(x^0) = a \exp(-m x^0)$$

- Perturbative expansion in $\Delta\varepsilon$:

$$a = a^{(0)} + \sum_l \Delta\varepsilon_l a_l^{(1)} + O(\Delta\varepsilon^2) \qquad m = m^{(0)} + \sum_l \Delta\varepsilon_l m_l^{(1)} + O(\Delta\varepsilon^2)$$

$$C(x^0) = C^{(0)}(x^0) + \sum_l \Delta\varepsilon_l C_l^{(1)}(x^0) + O(\Delta\varepsilon^2)$$

- $m^{(0)}$ and $a^{(0)}$ from non-linear fit to $O(\Delta\varepsilon^0)$ contribution:

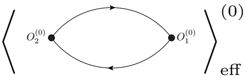
$$C^{(0)}(x^0) = a^{(0)} \exp(-m^{(0)} x^0)$$

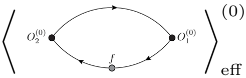
- $a_l^{(1)}$ and $m_l^{(1)}$ from linear fit to $O(\Delta\varepsilon^1)$ contribution:

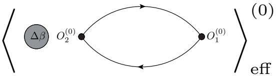
$$\frac{C_l^{(1)}(x^0)}{C^{(0)}(x^0)} = \frac{a_l^{(1)}}{a^{(0)}} - m_l^{(1)} x^0$$

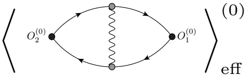
Mass splittings and averages of pseudo-scalar meson isospin multiplets

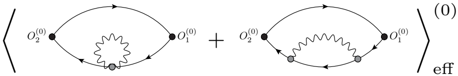
- Quark-connected contributions:

$C^{(0)}_{\mathrm{con}} =$ 

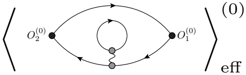
$C^{(1)}_{\Delta \mathrm{m}_f,\mathrm{con},\mathrm{det1}} =$ 

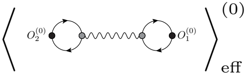
$C^{(1)}_{\Delta\beta,\mathrm{con},\mathrm{beta}} =$ 

$C^{(1)}_{\mathrm{e}^2,\mathrm{con},\mathrm{exch}} =$ 

$C^{(1)}_{\mathrm{e}^2,\mathrm{con},\mathrm{self1}} =$ 

- Quark-disconnected photon-connected contributions:

$C^{(1)}_{\mathrm{e}^2,\mathrm{con},\mathrm{vacexch1}} =$ 

$C^{(1)}_{\mathrm{e}^2,\mathrm{dis},\mathrm{exch}} =$ 

- Quark-disconnected photon-disconnected contributions:
  Absent for mass splittings, neglected for mass averages

Simulation details

$N_\mathrm{f} = 2+1$ gauge ensembles from CLS effort [Bruno et al., 2015, Bruno et al., 2017]:

- QCD gauge action: Tree-level improved Lüscher-Weisz action
- Quark action: O(a) improved Wilson fermions
- Boundary conditions: open in temporal direction, periodic in spatial directions
- Approach physical point on a trajectory with $\mathrm{Tr}(M) = \mathrm{const}$

	H102	H105
$\mathrm{T}/a \times (\mathrm{L}/a)^3$	96×32^3	96×32^3
β	3.4	3.4
a[fm]	0.08636(98)(40)	0.08636(98)(40)
m_π[MeV]	350	280
m_K[MeV]	440	460
$m_\pi L$	4.9	3.9

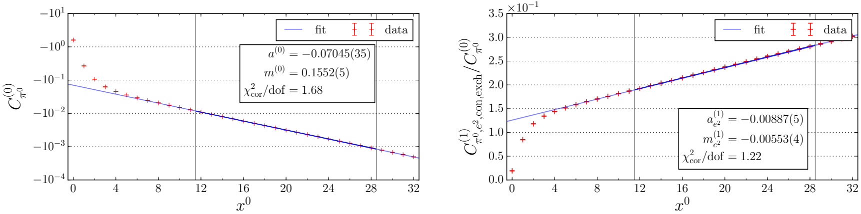
Measurement setup:

- measurements on 1000 configurations
- 4 $U(1)$ quark sources for connected part at timeslices 32 (forward) and 63 (backward)
- $4 \cdot 2$ Z_2 photon sources
- $4 \cdot 8$ $U(1)$ quark sources for disconnected part
- $4 \cdot 29$ inversions per configuration ($4 \cdot 5$ inversions for connected part)

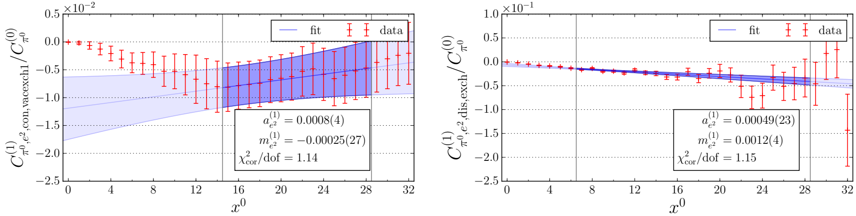
Mass splittings and averages of pseudo-scalar meson isospin multiplets

Examplary contributions for π^0 on H102 (preliminary):

- Quark-connected contributions:



- Quark-disconnected photon-connected contributions:



Contributions to π mass splitting and average

- H102 ($m_\pi = 350\text{MeV}$, $m_K = 440\text{MeV}$) (preliminary):

$m^{(0)}_{\pi^+}$	$m^{(0)}_{\pi^0}$
0.1552(5)	

diagram	par	$m^{(1)}_{\pi^+}$	$m^{(1)}_{\pi^0}$
con, det1	Δm_{u}	4.923(31)	2.461(16)
con, det2			
con, det1	Δm_{d}		
con, det2		4.923(31)	
con, beta	$\Delta\beta$	−10.9(1.2)	
con, self1	e^2	0.4529(28)	0.2831(18)
con, self2		0.1132(7)	
con, vacexch1		−0.0010(11)	−0.00025(27)
con, vacexch2		0.0005(5)	
con, exch		0.004473(24)	−0.00553(4)
dis, exch			0.0012(4)

  - con,vacexch-contributions vanish within errors
  - mass splitting given by con,exch- and dis,exch-contributions
  - dis,exch-contribution not negligible for mass splitting
  - $m_{\pi^+} - m_{\pi^0} = 1.688(201)_{\mathrm{st}}(21)_a\text{MeV}$ (fit to summed contributions)
- H105 ($m_\pi = 280\text{MeV}$, $m_K = 460\text{MeV}$) (preliminary):
  - con,vacexch-contributions vanish within errors
  - dis,exch-contribution comparably relevant for mass splitting
  - $m_{\pi^+} - m_{\pi^0} = 2.321(190)_{\mathrm{st}}(28)_a\text{MeV}$ (fit to summed contributions)
- From experiment: $m_{\pi^+} - m_{\pi^0} = 4.5936(5)\text{MeV}$

Contributions to K mass splitting and average

- H102 ($m_\pi = 350\text{MeV}$, $m_K = 440\text{MeV}$) (preliminary):

$m^{(0)}_{K^+}$	$m^{(0)}_{K^0}$
0.1921(4)	

diagram	par	$m^{(1)}_{K^+}$	$m^{(1)}_{K^0}$
con, det1	Δm_u	3.889(19)	
con, det2	Δm_d		3.889(19)
con, det2	Δm_s	3.955(10)	
con, beta	$\Delta\beta$	−9.7(1.0)	
con, self1	e^2	0.3585(17)	0.0896(4)
con, self2		0.09174(23)	
con, vacexch1		0.0001(8)	−0.0000(4)
con, vacexch2		0.0000(4)	
con, exch		0.003979(20)	−0.001990(10)

  - con,vacexch-contributions vanish within errors
  - mass splitting given by con,det1-, con,det2-, con,self1-, con,exch- and con,vacexch1-contributions

- H105 ($m_\pi = 280\text{MeV}$, $m_K = 460\text{MeV}$) (preliminary):
  - con,vacexch-contributions vanish within errors

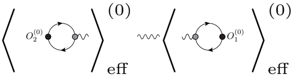
Summary and Future work

Summary:

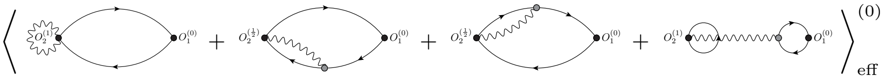
- Formulation of $\mathrm{QED_L}$ on open boundaries
- Construction of photon propagator in Coulomb gauge
- Relevance of quark-disconnected photon-connected contributions to pseudo-scalar meson masses

Future work:

- Hierarchical probing for estimation of disconnected quark loop
- Determination of isospin breaking effects in HVP for muon $g - 2$ [Blum et al., 2018]:



- Implementation of point-split (conserved) vector-current at sink [Boyle et al., 2017]:



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