QED in Weak Decays, Edinburgh 2022

QCD+QED on the lattice with C* boundary conditions

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RC*RC collaboration

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previously: M. Hansen, B. Lucini, A. Ramos

Charged states in a finite box

- A finite volume is needed in lattice simulations.
- Translational invariance is preserved in a finite box with periodic boundary conditions

$$A_\mu(t, \mathbf{x} + L\mathbf{k}) = A_\mu(t, \mathbf{x})$$

- Gauss law forbids states with nonzero charge in a periodic box

$$Q = \int_0^L d^3x \; j_0(t, \mathbf{x}) = \int_0^L d^3x \; \partial_k E_k(t, \mathbf{x}) = 0$$

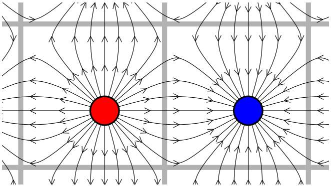
- Solutions discussed in this workshop:
  - change boundary conditions;
  - consider a massive photo (Della Morte);
  - break Gauss law by removing zero modes of the gauge field (Sachrajda, Hermansson-Truedsson);
  - consider QED in infinite volume (Jin).
- $C^\star$ (or C-periodic) boundary conditions represent the only option if you want preserve locality, translational and gauge invariance.

C* boundary conditions

Wiese, Nucl. Phys. B **375**, 45 (1992)
Polley, Z. Phys. C **59**, 105 (1993)
Kronfeld and Wiese, Nucl. Phys. B **357**, 521 (1991)
Lucini *et al.*, JHEP **1602**, 076 (2016)

Fields are periodic up to charge conjugation:

$$A_\mu(t, \mathbf{x} + L\mathbf{k}) = -A_\mu(t, \mathbf{x})$$
$$B_\mu(t, \mathbf{x} + L\mathbf{k}) = -B_\mu^*(t, \mathbf{x})$$
$$\psi(t, \mathbf{x} + L\mathbf{k}) = C^{-1}\bar{\psi}^T(t, \mathbf{x})$$



Flux of electric field across the boundaries is not forced to vanish

$$Q(t) = \int d^3x\, j_0(t, \mathbf{x}) = \int d^3x\, \partial_k E_k(t, \mathbf{x}) \neq 0$$

The charge is locally conserved, but not globally: it can flow outside of the box. This is analogous to the physical situation in infinite volume in which one measures the charge only in a finite volume.

- On-shell Ward identities $\langle \psi_1 | \partial_\mu j^\mu(x) | \psi_2 \rangle = 0$.
- Global $U(1)$ broken to $\mathbb{Z}_2$.

Gauge invariant interpolating operators

- In infinite volume, a charged pion can be created with the following **gauge invariant** operator:

$$e^{-i \frac{1}{\nabla^2} \nabla \mathbf{A}(t,\mathbf{x})} \bar{u}\gamma_5 d(t, \mathbf{x}) = e^{-i \int d^3y \, \phi(\mathbf{x}-\mathbf{y}) \nabla \mathbf{A}(t,\mathbf{y})} \bar{u}\gamma_5 d(t, \mathbf{x})$$

  where ϕ is the Coulomb potential. These operators create a pion with its own Coulomb field.

  P. Dirac, *Gauge invariant formulation of quantum electrodynamics*, Can. J. Phys. **33** (1955), 650.

- In finite volume with C* boundary conditions these operators are constructed in the same way: ϕ is the Coulomb potential with antiperiodic boundary conditions.

- Why do we care about gauge invariance? Using covariant gauges with gauge-variant operators is a bad idea!

$$\langle \Omega | C^\dagger e^{-tH} C | \Omega \rangle = \sum_{\text{physical states}} + \sum_{\text{unphysical states}} |\langle \psi_n | C | \Omega \rangle|^2 \, e^{-tE_n}$$

  e.g. in the Gupta-Bleuler formalism, physical states satisfy $\partial^\mu A^+_\mu(x)|\psi\rangle = 0$.

- Unphysical states do not appear when gauge-invariant operators are used (or if one works in Coulomb gauge).

Two strategies for QCD+QED: RM123 method

de Divitiis *et al.* [RM123], *Leading isospin breaking effects on the lattice*, Phys.Rev. D87 (2013) 11, 114505.

- Expand action in powers of eA_μ (the photon field appears non linearly in the lattice-discretized interaction action):

$$S_{\text{QCD+QED}} = S_{\text{QCD}} + S_\gamma + e \sum_{x\mu} A_\mu(x) J_\mu(x) + e^2 \sum_{xy\mu\nu} A_\mu(x) A_\nu(y) T_{\mu\nu}(x,y) + O(e^3)$$

- Expand expectation values in powers of e, e.g. if O does not depend on A:

$$\langle O \rangle_{\text{QCD+QED}} = \langle O \rangle_{\text{QCD}} + \frac{e^2}{2} \sum_{xy\mu} D(x,y) \langle O J_\mu(x) J_\mu(y) \rangle_{\text{QCD},c} - e^2 \sum_{xy\mu} D(x,y) \langle O T_{\mu\nu}(x,y) \rangle_{\text{QCD},c} + O(e^4)$$

- Calculate the coefficients of the expansion with QCD simulations.

Two strategies for QCD+QED: full simulations

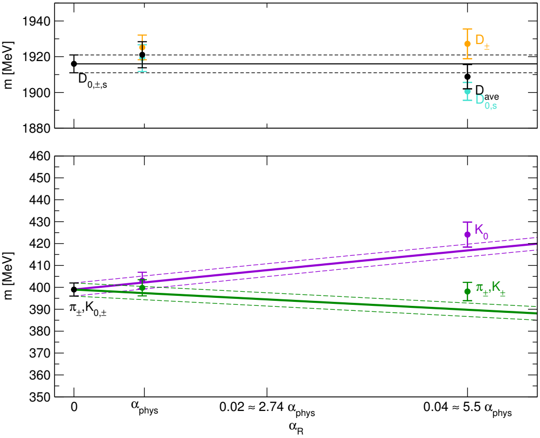
Borsanyi *et al.* [BMW], *Ab initio calculation of the neutron-proton mass difference*, Science 347 (2015) 1452-1455.

R. Horsley *et al.* [CSSM, QCDSF and UKQCD], *Isospin splittings in the decuplet baryon spectrum from dynamical QCD+QED*, J. Phys. G **46** (2019), 115004.

- Simulate QCD+QED at several values of α_{em}, including $\alpha_{em} = 0$, then interpolate to $\alpha_{em} = 1/137$.

- We are currently using this approach. However in the long term we plan to make a detailed comparison of the two methods.

Overview of simulations



scale fixed with the conventional value
$\sqrt{8t_0} = 0.415$ fm

fixed $\beta = 3.24$ correspoding to
$a \simeq 0.05$ fm

64×32^3 lattice corresponding to
$M_{\pi_\pm} L \simeq 3.3$

m_u, $m_d = m_s$, m_c are tuned to

$M^2_{\pi_\pm} + M^2_{K_\pm} + M^2_{K_0} \simeq$ PDG value

$\alpha_R^{-1}(M^2_{K_0} - M^2_{K_\pm}) \simeq$ PDG value

$M_{D_\pm} + M_{D_0} + M_{D_s} \simeq$ PDG value

Mistuning is corrected by means of mass reweighting.

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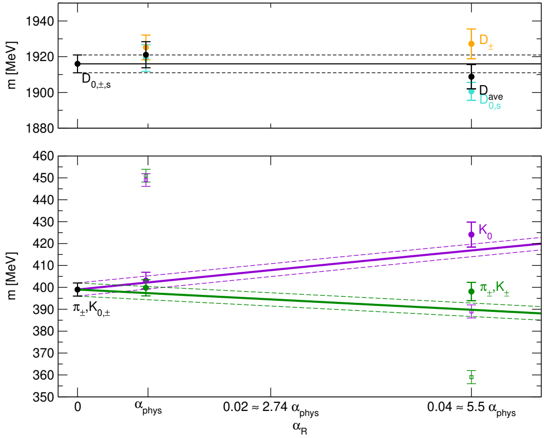

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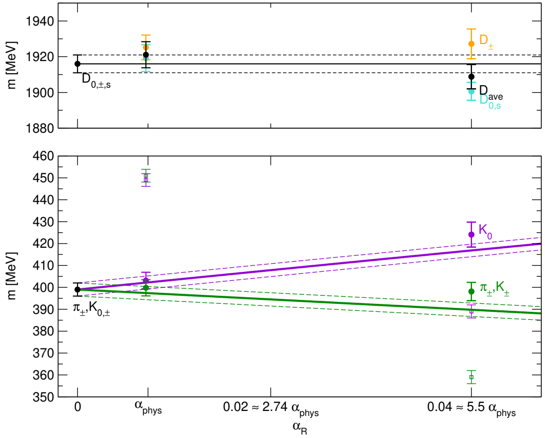

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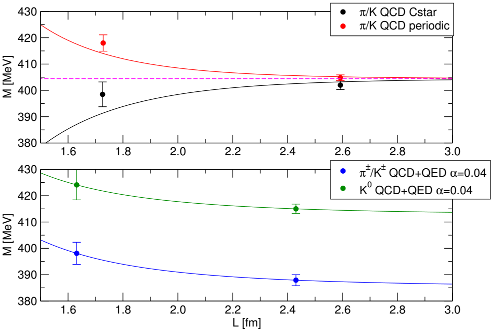
$$M_{D_\pm} + M_{D_0} + M_{D_s} \simeq \text{PDG value}$$

Mistuning is corrected by means of mass reweighting.

α_R	$M_{K^0} - M_{K^\pm}$	$M_{D^\pm} - M_{D^0}$ [MeV]
α_{phys}	4.26(41)	6.3(1.6)
$5.5\alpha_{phys}$	25.8(4.5)	27.6(8.0)

Finite volume effects

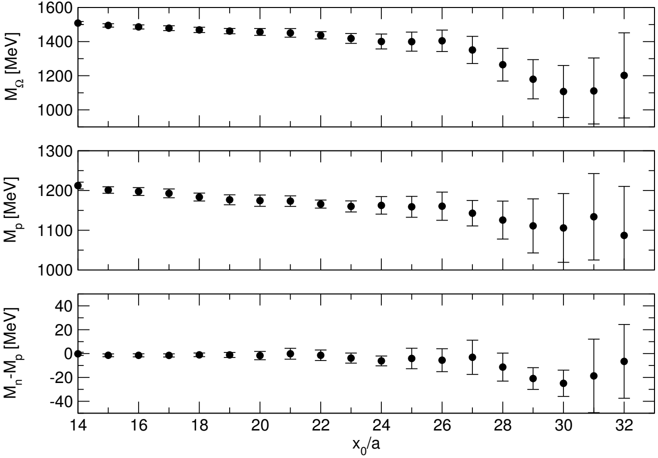


- QCD with periodic boundary conditions from: R. Höllwieser *et al.* [ALPHA], *Scale setting for $N_f = 3+1$ QCD*, Eur. Phys. J. C **80** (2020) no.4, 349.
- QCD fits to LO χPT. Simulations at $M_\pi L \simeq 3.3$ and $M_\pi L \simeq 4.9$.
- QED finite volume effects:

$$M(L) = M(\infty) - \alpha_R \left\{ \frac{q^2\, 1.748\ldots}{2L} + \frac{q^2\, 2.519\ldots}{\pi M(\infty) L^2} + O\left(\frac{1}{L^4}\right) \right\}$$

- Finite volume effects are unsurprisingly too big on our small volume.

Baryons



M_Ω [MeV]
1600
1400
1200
1000
M_p [MeV]
1300
1200
1100
1000
M_n-M_p [MeV]
40
20
0
-20
-40
14
16
18
20
22
24
26
28
30
32
x_0/a

Some technical details

- Compact formulation of QED: fundamental variables are the parallel transports between nearest neighbours on the lattice $z_\mu(x) = e^{iaq_{el}A_\mu(x)}$. Action:

$$S_\gamma = \frac{1}{8\pi q_{el}^2\alpha} \sum_{x\mu\nu} [1 - z_{\mu\nu}(x)]$$

In practice, we are always in the deep perturbative regime, e.g.

ensemble	α	$q_{el}^2\alpha$	U(1) plaquette
A380a07b324	0.007299	0.00020275	$1 - 6.33184(11) \times 10^{-4}$
A360a50b324	0.050000	0.00138889	$1 - 4.19405(21) \times 10^{-3}$

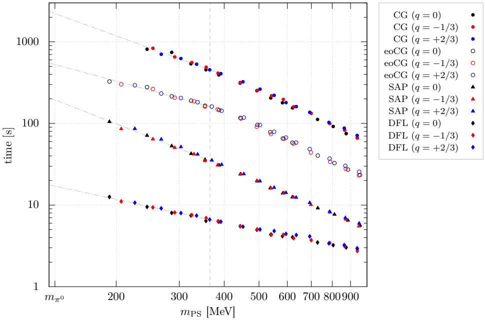
Why? Straightforward implementation, no need to fix the gauge at any stage, out-of-the box compatibility with all temporal boundary conditions of `openQCD`.

- Lüscher-Weisz SU(3) gauge action.

- Dirac-Wilson fermions with SW term for SU(3) and U(1) field with $c_{sw,SU(3)}$ determined non-perturbatively in QCD and $c_{sw,U(1)} = 1$.

Some technical details

- Because of C* boundary conditions, we need to calculate the Pf(CKD). We always include the sign of the Pfaffian in our results.
- RHMC used for all quarks.
- Light-quark Dirac operator inverted with Generalized Conjugate Residue Method + Schwarz Alternating Procedure Preconditioner + Lüscher's Inexact Deflation (GCR+SAP+DFL).



Cost of simulations

α_R	N_f	a[fm]	M_π [MeV]	acc.	τ_{exp}[MDU]	core × hours/MDU	
0	3+1	0.05	400	95%	102(36)	242	RC*, HLRN Lise
1/137	1+2+1	0.05	380	92%	92(30)	599	"
0.04	1+2+1	0.05	360	95%	94(38)	616	"
0	2+1	0.05	420	95%	∼110(40)	99	rescCLS, SuperMUC
0	2+1	0.086	350	97%	∼40(10)	137	"

Conclusions

- C* boundary conditions provide the only option for QED in finite volume, if you want to preserve locality, gauge inveriance and translational invariance.
- QED corrections to hadronic observables can be calculated on the lattice by means of a perturbative expansion in α_{em} (only QCD needs to be simulated), or by simulating the full theory (QCD+QED).
- The RC* collaboration is investigating the second option. We have generated configurations with $m_d = m_s$, $\alpha = 0, 1/137, 0.04$ and $a \simeq 0.05$ fm.
- Is simulating QCD+QED the best option? A detailed comparison with the RM123 method is under way.
- The tuning of quark masses is particularly painful, but we managed to reduce the pain by using mass reweighting.
- Finite volume effects are unsurprisingly too big on our small volume, but the large volume seems OK. More studies are needed.
- We are calculating baryon masses; some preliminary results are available.