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Isospin-breaking effects with C^* boundary conditions

RGXO₂ collaboration

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Introduction

- \triangleright Isospin transformations (i.e. unitary transformations of the up/down doublet) are are approximated symmetries of Nature.
- **I** Isospin symmetry is broken by $m_u \neq m_d$ and $q_u \neq q_d$.
- \triangleright Isospin-breaking effects are typically of order 1% on hadronic observables.
- \blacktriangleright In order to calculate hadronic observables at the percent or subpercent precision level, one needs to consider QCD+QED.

Introduction

- \triangleright Often, electroquenched approximation (i.e. valence quarks are charged, sea quarks are neutral)! We need to do better.
- Including the sea-quark effects is difficult. Full simulations or RM123 method?
- RC^{*} collaboration: full QCD+QED simulations with C^* boundary conditions.
- \triangleright RC* collaboration: on-going detailed study of variance of sea-quark effects in RM123 method.

(Quick) theoretical intro

Two ways for QCD+QED on the lattice

1. RM123 method

G. M. de Divitiis *et al.* [\[RM123\], "Leading isospin breaking...," Phys.Rev.D 87 \(2013\) 11, 114505.](https://inspirehep.net/literature/1224545)

$$
S_{\text{QCD+QED}} = S_{\text{QCD}} + S_{\gamma} + \frac{\delta \beta}{\beta} S_{\text{gluon}} + \sum_{xf} \delta m_f \, \bar{\psi}_f \psi_f(x) + e \sum_{x\mu} A_{\mu}(x) \mathcal{J}_{\mu}(x) + e^2 \sum_{x\mu} A_{\mu}(x)^2 \mathcal{T}_{\mu}(x) + O(e^3)
$$

Pros:

- \triangleright Calculate directly isospin-breaking and radiative correction to QCD (10%) precision is enough).
- \triangleright Reuse QCD configurations (careful with the finite-volume effects).
- \triangleright Tuning is trivial: QED counterterms are calculated by solving linear equations.

Cons:

- \triangleright Complicated observables, quark-disconnected pieces, expensive variance-reduction techniques.
- \triangleright Correction-to-QCD noise ratio diverges with $V^{1/2}$ and a^{-2} . Bad scaling with *V* can be killed with coordinate-space techniques, bad scaling with *a* is irreducible.

Two ways for QCD+QED on the lattice 2. QCD+QED simulations

Gluon and photon fields are treated on equal footing. Fully interacting $SU(3) \times U(1)$ configurations are generated. Used in:

S. Borsanyi *et al.* [\[BMW\], "Ab initio calculation...," Science 347 \(2015\), 1452-1455.](https://inspirehep.net/literature/1300659)

R. Horsley *et al.* [QCD-SF], "QED eff[ects...," JHEP 04 \(2016\), 093.](https://inspirehep.net/literature/1391515) R. Horsley *et al.* [\[QCD-SF\],](https://inspirehep.net/literature/1389860) ["Isospin splittings of meson and baryon masses...," J.Phys.G 43 \(2016\) 10, 10LT02.](https://inspirehep.net/literature/1389860)

A. Altherr *et al.* [\[RC*\], "First results on QCD+QED with C](https://inspirehep.net/literature/2157207)^{*} boundary conditions," JHEP 03 [\(2023\), 012, 1452-1455.](https://inspirehep.net/literature/2157207)

Pros:

- \triangleright Standard algorithms can be used.
- \blacktriangleright Simpler observables.
- ▶ The scaling of the noise in QCD+QED with *V* and *a* is like in QCD.

Cons:

- \blacktriangleright Expensive simulations.
- \triangleright Observables need to be calculated at the permille precision level.
- \blacktriangleright Up and down quark masses need to be tuned independently.

Charged states

The Gauss's law forbids charged states with periodic boundary conditions:

$$
Q = \int_0^L d^3x \, \rho(\mathbf{x}) = \int_0^L d^3x \, \nabla \cdot \mathbf{E}(\mathbf{x}) = 0 \; .
$$

Some popular solutions:

- ▶ QED_L: non-local constraint $\int d^3x A_\mu(t, x) = 0$.
- \blacktriangleright QED_m: massive photon.
- \triangleright QED_{∞}: (only with RM123) reconstruct infinite-volume QCD *n*-point functions and integrate them with infinite-volume photon propagators.
- \blacktriangleright QED_C: C-periodic boundary conditions in space $\phi(t, x + Le_k) = \phi^C(t, x)$.

Some properties of QED_C :

- \triangleright Continuum limit described by Symanzik effective theory (like QED_{m}).
- E Leading finite-volume effects dominated by low-energy states (like QED_m).
- ▶ Power-like finite-volume effects to single-particle masses and matrix elements (like $QED₁$).
- Incompatible with θ -periodic boundary conditions.
- **Partially-broken flavour symmetry.**

Full QCD+QED simulations

openQ*D code

<https://gitlab.com/rcstar/openQxD>

- Extension of openQCD-1.6
- \triangleright Simulation of QCD and QCD+QED
- \blacktriangleright C^{*} boundary conditions in space
- \blacktriangleright Compact photon action
- \blacktriangleright Wilson flow for photon field
- \blacktriangleright Fourier acceleration for photon field
- \blacktriangleright Multiple deflation subspaces
- \blacktriangleright U(1)-invariant quark propagators

[See talk at Lattice2024: Roman Gruber,](https://conference.ippp.dur.ac.uk/event/1265/contributions/7350/) *O*(*a*)-improved QCD+QED Wilson Dirac [operator on GPUs, Software Development and Machines, 30 July 2024 14:25](https://conference.ippp.dur.ac.uk/event/1265/contributions/7350/)

I. Campos *et al.*[, "openQ*D code: a versatile tool for QCD+QED simulations," Eur.Phys.J.C 80](https://inspirehep.net/literature/1751937) [\(2020\) 3, 195.](https://inspirehep.net/literature/1751937)

openQ*D code

<https://gitlab.com/rcstar/openQxD>

Coming up (testing phase):

- \blacktriangleright Sign of determinant/Pfaffian
- \blacktriangleright Mass reweighting
- Interface to QUDA solvers

 \blacktriangleright Various noise-reduction techniques for RM123 method (hopping expansion, frequency splitting, truncated solvers, expandable...)

[See talk at Lattice2024: Roman Gruber,](https://conference.ippp.dur.ac.uk/event/1265/contributions/7350/) *O*(*a*)-improved QCD+QED Wilson Dirac [operator on GPUs, Software Development and Machines, 30 July 2024 14:25](https://conference.ippp.dur.ac.uk/event/1265/contributions/7350/)

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Ensembles

Meson masses

$$
\phi_0 = 8t_0(M_{K\pm}^2 - M_{\pi\pm}^2) = 0 \qquad \phi_2 = 8t_0\alpha_R^{-1}
$$

$$
\phi_1 = 8t_0(M_{\pi\pm}^2 + M_{K\pm}^2 + M_{K_0}^2) \simeq \phi_1^{\text{phys}} \qquad \phi_3 = \sqrt{8t_0}(I)
$$

$$
\phi_2 = 8t_0 \alpha_R^{-1} (M_{K_0}^2 - M_{K^\pm}^2) \simeq \phi_2^{\text{phys}}
$$

$$
\phi_3 = \sqrt{8t_0} (M_{D_0} + M_{D^\pm} + M_{D_s^\pm}) \simeq \phi_3^{\text{phys}}
$$

Meson masses

$$
M(L) = M(\infty) - \frac{\alpha_R q^2 c_1}{2L} - \frac{\alpha_R q^2 c_2}{2ML^2} + O\left(\frac{1}{L^4}\right)
$$

Universal FV correction for K^{\pm} at $\alpha_R \simeq 5.6 \alpha_{\text{phys}}$ $L/a = 32$: 1.09(1)% + 0.308(8)% $L/a = 48$: $0.751(4)\% + 0.145(2)\%$

 $a \simeq 0.05$ fm $\alpha_R \simeq 0.04$ *M*_{$\pi \pm$} $\simeq 400$ MeV *M*_{$\pi \pm$} $L \simeq 4$

2000 configurations, 4 stochastic sources per configuration, smearing

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Isospin-breaking corrections to HVP

In all cases, tails are fitted to a single exponential after \sim 1.2 fm.

[See talk at Lattice2024: Letizia Parato, Update on the isospin breaking corrections to](https://conference.ippp.dur.ac.uk/event/1265/contributions/7447/) [the HVP with C-periodic boundary conditions, Hadronic and nuclear spectrum and](https://conference.ippp.dur.ac.uk/event/1265/contributions/7447/) [interactions, 1 August 2024 12:10](https://conference.ippp.dur.ac.uk/event/1265/contributions/7447/)

Isospin-breaking corrections to HVP

- 1. Corrections from Z $\delta Z_V a_\mu^{\text{HVP}, u} = (-510(32)\Delta m_u - 22(3)e^2) \times 10^{-10}$ $\delta Z_V a_\mu^{\text{HVP}}, d/s = (-128(8)\Delta m_d - 1.4(2)e^2) \times 10^{-10}$ δZ_V a $_{\mu}^{\rm HVP, c} = (-6.37(2)\Delta m_c - 0.578(2)e^2) \times 10^{-10}$
- 2. Corrections from *G*

 \blacktriangleright $G''(t)$ – local-local case

$$
\delta_G a_\mu^{HVP, u} = (-4364(266)\Delta m_u - 216(14)e^2) \times 10^{-10}
$$

$$
\delta_G a_\mu^{HVP, d/s} = (-1091(67)\Delta m_d - 13.5(9)e^2) \times 10^{-10}
$$

$$
\delta_G a_\mu^{HVP, c} = (-59.2(3)\Delta m_c - 3.119(13)e^2) \times 10^{-10}
$$

►
$$
G^{cl}(t)
$$
 – conserved-local case
\n
$$
\delta_G a_H^{HVP,u} = (-4591(288)\Delta m_u - 227(15)e^2) \times 10^{-10}
$$

$$
\delta_G a_\mu^{HVP, d/s} = (-1148(72)\Delta m_d - 14.2(1.0)e^2) \times 10^{-10}
$$

$$
\delta_G a_\mu^{HVP, c} = (-57.2(2)\Delta m_c - 3.295(14)e^2) \times 10^{-10}
$$

 δa_{μ} from G larger than those from Z

Derivatives of *Zv*(8*,* 8) (left) and mixed components *Zv*(8*,* 0), *Zv*(8*,* 3), *Zv*(8*,* 15) (right) over m_{II} (top) or α (bottom)

Derivatives of *G*up (top) and *G*charm (bottom) over lass (left) and α (right)

RM123 method

Expansion of Dirac operator

$$
D(e) = D(e = 0) + \delta m
$$

+ $i\frac{eq}{2}\sum_{\mu}(A_{\mu}H_{\mu} - \bar{H}_{\mu}A_{\mu})$
- $\frac{e^2q^2}{4}\sum_{\mu}(A_{\mu}^2H_{\mu} + \bar{H}_{\mu}A_{\mu}^2)$
- $\frac{eqc_{sw}U(1)}{4}\sum_{\mu\nu}\sigma_{\mu\nu}F_{\mu\nu}^{sym} - \frac{\delta c_{sw}^{SU(3)}}{4}\sum_{\mu\nu}\sigma_{\mu\nu}\widehat{G}_{\mu\nu}$
+ $O(e_0^3)$

Hopping operators:

$$
H_{\mu}\chi(x) = (1 - \gamma_{\mu})U(x, \mu)\chi(x + \hat{\mu}) \qquad \bar{H}_{\mu}\chi(x) = (1 + \gamma_{\mu})U(x - \hat{\mu}, \mu)^{\dagger}\chi(x - \hat{\mu})
$$

Expansion of Dirac operator

Expansion of Dirac operator					
$D(e) = D(e = 0) + \boxed{bm}$	$W3SS \text{ shift}$	$-\frac{1}{2}$			
$+ i\frac{eq}{2} \sum_{\mu} (A_{\mu}H_{\mu} - \bar{H}_{\mu}A_{\mu})$	$2\frac{3}{2}$				
$- \frac{e^{2}q^{2}}{4} \sum_{\mu} (A_{\mu}^{2}H_{\mu} + \bar{H}_{\mu}A_{\mu}^{2})$	$- \frac{1}{2}$				
$i\hbar \text{ of a point}$	$-\frac{2}{4} \sum_{\mu\nu} (A_{\mu}^{2}H_{\mu} + \bar{H}_{\mu}A_{\mu}^{2})$	$i\hbar \text{ of pole}$	$-\frac{1}{2}$		
$i\hbar \text{ of a point}$	$-\frac{1}{2}$				
$i\hbar \text{ of a point}$	$-\frac{1}{2}$				
$- \frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$- \frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$
$i\hbar \text{ of a$					

Hopping operators:

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H_{\mu}\chi(x) = (1 - \gamma_{\mu})U(x, \mu)\chi(x + \hat{\mu}) \qquad \bar{H}_{\mu}\chi(x) = (1 + \gamma_{\mu})U(x - \hat{\mu}, \mu)^{\dagger}\chi(x - \hat{\mu})
$$

Expansion of pion correlator

Divergence of variance

 \triangleright Consider the quantity at positive flowtime

$$
A(t,x) = \frac{t^2}{2} \text{tr} \,\hat{F}_{\mu\nu} \hat{F}_{\mu\nu}(t,x)
$$

- In QCD simulations, both $A(t, x)$ and its variance are finite in the $V \rightarrow +\infty$ and $a \rightarrow 0$ limits.
- In full QCD+QED simulations, both $A(t, x)$ and its variance are finite in the $V \rightarrow +\infty$ and $a \rightarrow 0$ limits.
- If *R* is one of the see diagrams of the RM123 method, and α is the configuration index, then the estimator for the RM123 insertion

$$
\frac{1}{N_g}\sum_{\alpha}A_{\alpha}(t,x)R_{\alpha}-\frac{1}{N_g(N_g-1)}\sum_{\alpha\neq\beta}A_{\alpha}(t,x)R_{\beta}
$$

has a variance that diverges like $V^{1/2}$ in the $V \rightarrow \infty$ limit and a^{-2} in the $a \rightarrow 0$ limit.

[See talk at Lattice2024: Alessandro Cotellucci, Error Scaling of Sea Quark](https://conference.ippp.dur.ac.uk/event/1265/contributions/7448/) Isospin-Breaking Eff[ects, Hadronic and nuclear spectrum and interactions, 1 August](https://conference.ippp.dur.ac.uk/event/1265/contributions/7448/) [2024 11:50](https://conference.ippp.dur.ac.uk/event/1265/contributions/7448/)

Summary

Full QCD+QED simulations:

- \triangleright Simulations run as well/bad as QCD ones. More expensive because of C^* boundary conditions and RHMC for all quarks.
- In Tuning of quark masses is difficult but not hopeless. Which precision do we need?
- ▶ Meson effective masses are obtained with a statistical precision similar to QCD. Finite-volume effects need to be quantified better.
- \triangleright We calculated *p*, *n*, Ξ^- , Λ_0 , Ω^- masses. Too noisy for now. We are neglecting extra Wick contractions due to C^* boundary conditions. We are working on it
- I We are calculating isospin-breaking corrections to HVP contribution to muon $g 2$ on QCD+QED configurations.

RM123 method:

- \blacktriangleright Reaching the gauge noise for the sea-quark insertions is painful but can be done.
- **I** Error of sea-quark insertions diverges asymptotically as $V^{1/2}$ and a^{-2} .
- In the considered range of parameters we see the $V^{1/2}$ quite well, while the lattice spacing behaviour seems better than the asymptotic one. More statistics is needed...
- \triangleright Good news: large cancellation of errors among various constributions. Needs more investigation...

Backup

IB corrections - Last updates from Zürich

RC* collaboration July 21, 2024

Comparing two methods for calculating Isospin Breaking Effects

Goal: Cross-validate and compare costs and challenges of two approaches to compute IB effects at fixed lattice spacing and volume:

- 1. Direct QCD+QED with dynamical $U(1)$ and $m_u \neq m_d$
- 2. **IsoQCD** + RM123: perturbative expansion in $m_d m_u$ and α_{QED} , including all sea effects

Setup: 2 ensembles with Wilson fermions, $O(a)$ improved action with coeff. $c_{\rm sw}^{\rm SU(3)}=2.18859$ and $c_{\rm sw}^{\rm U(1)}=1$, *same volume and* β , but *different* κ_q *and* α :

ensemble	lattice β		α	$\kappa_{\rm u}$	$\kappa_d = \kappa_s$	κ_c
A400a00b324 64×32^3 3.24				0 0.13440733 0.13440733		0.12784
$A380a07b324$ 64×32^3 3.24 0.007299 0.13457969 0.13443525						0.12806355
$\delta m_a = m_a^{\text{A380}} - m_a^{\text{A400}}$					$-0.00476435 - 0.000772590 - 0.00682735$	

Target observable: HVP contribution to $(g - 2)_{\mu}$.

Key steps:

- Compute all relevant observables at LO
- Correlator derivatives: $\partial G/\partial m_f$, $\partial G/\partial e^2$ and derivatives to Z_V (see next slide)
- \bullet Combine $\delta \vec{\epsilon} \equiv (\delta \beta, \delta \alpha, \delta m_u, \delta m_{d/s}, \delta m_c)$ and derivatives to get IB effects to $a_\mu^{\rm HVP}$

IB corrections to the HVP

Using the local-local implementation¹ for the correlator, $G^{\ell\ell}(t)$,

$$
a_{\mu}^{HVP} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^{\infty} dt \, Z_V^2 G^{\ell\ell}(t) \tilde{K}(t; m_{\mu}).
$$

 a_{μ}^{HVP} receives two types of IB corrections:

1. Corrections to the correlator:

$$
\delta a_{\mu,(1)}^{HVP} = \left(\frac{\alpha}{\pi}\right)^2 \int dt \left(Z_V^{(0)}\right)^2 \delta G^{\ell\ell}(t) \tilde{K}(t; m_\mu)
$$

$$
G^{\ell\ell}(t) = G^{\ell\ell}(t)^{(0)} + \delta G^{\ell\ell}(t) = G^{\ell\ell}(t)^{(0)} + \sum_f \delta m_f \left. \frac{\partial G^{\ell\ell}(t)}{\partial m_f} \right|_{(0)} + \frac{e^2}{2} \left. \frac{\partial^2 G^{\ell\ell}(t)}{\partial e^2} \right|_{(0)}
$$

2. Corrections to renormalization constants:

$$
\delta a_{\mu,(2)}^{HVP} = \left(\frac{\alpha}{\pi}\right)^2 \int dt \, 2Z_V^{(0)} \delta Z_V G^{\ell\ell}(t)^{(0)} \tilde{K}(t; m_\mu)
$$

$$
Z_V = Z_V^{(0)} + \delta Z_V = Z_V^{(0)} + \sum_f \delta m_f \frac{\partial Z_V}{\partial m_f} \bigg|_{(0)} + \frac{1}{2} e^{2} \frac{\partial^2 Z_V}{\partial e^2} \bigg|_{(0)}
$$

Alternatively, we also use conserved-local correlator $G^{c\ell}(t).$

Shifts of bare parameters $(e^2, \delta m_u, \ldots, \delta m_c)$ fixed to $\delta \epsilon_i = \epsilon_i^{A380$ a07 | {z } *QCD*+*QED* $-\frac{\epsilon}{2}$ A400a00 *i* | {z } *IsoQCD*

RM123: Diagrams for leading IB effects (connected valence only here)

Derivatives from our action $S^{QCD+QED+SW} = S_f(e, m_f) + S_{SW}(e) + \delta Sb$

With $\mathcal{G}^{c\ell}(t)$, if conserved current $V_\mu^c(\mathsf{x})$ defined at the sink, no additional propagators needed, but two additional diagrams appear:

Renormalization constants Z_V and their IB corrections

Renormalization condition in the adjoint basis of the identity λ_0 plus SU(4) generators $\lambda_3, \lambda_8, \lambda_{15}$:

$$
Z_{V_RV_I} = \lim_{x_0 \to \infty} G^{cl}(x_0) (G^{\ell\ell}(x_0))^{-1} \to \left(\begin{smallmatrix} 0.6578(9) & 0.0(0) & 0.0(0) & 0.0220(6) \\ 0.0(0) & 0.6766(12) & 0.0(0) & 0.0(0) \\ 0.0(0) & 0.0(0) & 0.0(0) & 0.0(0) \\ 0.0439(12) & 0.0(0) & 0.0(0) & 0.6224(11) \end{smallmatrix} \right)
$$

Taking derivatives:

$$
\frac{\partial Z_{V_R V_I}}{\partial \varepsilon_i} = \lim_{x_0 \to \infty} \left[\frac{\partial G^{cl}}{\partial \varepsilon_i}(x_0) - G^{cl}(x_0) (G^{\ell \ell}(x_0))^{-1} \frac{\partial G^{\ell \ell}}{\partial \varepsilon_i}(x_0) \right] \cdot (G^{\ell \ell}(x_0))^{-1}
$$

Total correction:

$$
\delta Z_{V_R V_I} = \sum_f \Delta m_f \frac{\partial Z_{V_R V_I}}{\partial m_f} + e^2 \frac{\partial Z_{V_R V_I}}{\partial e^2} + \dots
$$

Using mass shifts:

$$
\delta Z_{V_RV_I} = \begin{pmatrix} -0.00002(19) & 0.000260(95) & 0.00027(11) & 0.000147(76) \\ 0.000230(93) & -0.00008(16) & 0.00027(11) & 0.000094(38) \\ 0.000133(54) & 0.00027(11) & -0.00005(19) & 0.000054(22) \\ 0.00030(15) & 0.00038(15) & 0.000217(87) & -0.000259(62) \end{pmatrix}
$$

Results for $a_{\mu}^{\rm HVP}$ from LO connected correlators

In all cases, tails are fitted to a single exponential after \sim 1.2 fm.