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Isospin-breaking effects with C^{\star} boundary conditions

RC*ON collaboration

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CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre



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Special Article - Tools for Experiment and Theory	
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Introduction

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

Introduction

- 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.
- 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.

$$S_{\text{QCD+QED}} = S_{\text{QCD}} + S_{\gamma} + \frac{\delta\beta}{\beta} S_{gluon} + \sum_{xf} \delta m_f \, \bar{\psi}_f \psi_f(x)$$

+ $e \sum_{x\mu} A_{\mu}(x) \mathcal{J}_{\mu}(x) + e^2 \sum_{x\mu} A_{\mu}(x)^2 \mathcal{T}_{\mu}(x) + O(e^3)$

Pros:

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

Cons:

- Complicated observables, quark-disconnected pieces, expensive variance-reduction techniques.
- 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.

R. Horsley *et al.* [QCD-SF], "QED effects...," JHEP 04 (2016), 093. R. Horsley *et al.* [QCD-SF], "Isospin splittings of meson and baryon masses...," J.Phys.G 43 (2016) 10, 10LT02.

A. Altherr *et al.* [RC*], "First results on QCD+QED with C* boundary conditions," JHEP 03 (2023), 012, 1452-1455.

Pros:

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

Cons:

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

Charged states

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

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

Some popular solutions:

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

Some properties of QED_C:

- Continuum limit described by Symanzik effective theory (like QED_m).
- 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 QED_L).
- Incompatible with θ -periodic boundary conditions.
- Partially-broken flavour symmetry.

Full QCD+QED simulations

openQ*D code

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https://gitlab.com/rcstar/openQxD

- Extension of openQCD-1.6
- Simulation of QCD and QCD+QED
- C* boundary conditions in space
- Compact photon action

- Wilson flow for photon field
- Fourier acceleration for photon field
- Multiple deflation subspaces
- U(1)-invariant quark propagators

See talk at Lattice2024: Roman Gruber, O(a)-improved QCD+QED Wilson Dirac operator on GPUs, Software Development and Machines, 30 July 2024 14:25

I. Campos *et al.*, "openQ*D code: a versatile tool for QCD+QED simulations," Eur.Phys.J.C 80 (2020) 3, 195.

openQ*D code



https://gitlab.com/rcstar/openQxD

Coming up (testing phase):

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

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

See talk at Lattice2024: Roman Gruber, O(a)-improved QCD+QED Wilson Dirac operator on GPUs, Software Development and Machines, 30 July 2024 14:25

I. Campos *et al.*, "openQ*D code: a versatile tool for QCD+QED simulations," Eur.Phys.J.C 80 (2020) 3, 195.

Ensembles



Meson masses



$$\begin{split} \phi_0 &= 8t_0(M_{K^{\pm}}^2 - M_{\pi^{\pm}}^2) = 0\\ \phi_1 &= 8t_0(M_{\pi^{\pm}}^2 + M_{K^{\pm}}^2 + M_{K_0}^2) \simeq \phi_1^{\mathsf{phys}} \end{split}$$

$$\begin{split} \phi_2 &= 8t_0 \alpha_R^{-1} (M_{K_0}^2 - M_{K^{\pm}}^2) \simeq \phi_2^{\text{phys}} \\ \phi_3 &= \sqrt{8t_0} (M_{D_0} + M_{D^{\pm}} + M_{D_s^{\pm}}) \simeq \phi_3^{\text{phys}} \end{split}$$

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 $\alpha_R \simeq 5.6 \alpha_{phys}$ L/a = 32: 1.09(1)% + 0.308(8)%L/a = 48: 0.751(4)% + 0.145(2)%



 $a\simeq 0.05 {
m fm}$ $lpha_R\simeq 0.04$ $M_{\pi^\pm}\simeq 400 {
m MeV}$ $M_{\pi^\pm}L\simeq 4$

2000 configurations, 4 stochastic sources per configuration, smearing



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See poster at Lattice2024: Sara Rosso, Partially connected contributions to baryon masses in QCD+QED, 30 July 2024 18:15



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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 the HVP with C-periodic boundary conditions, Hadronic and nuclear spectrum and interactions, 1 August 2024 12:10

Isospin-breaking corrections to HVP

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

2. Corrections from G

G^{II}(t) – local-local case

$$\begin{split} &\delta_{G}a_{\mu}^{HVP,u} = (-4364(266)\Delta m_{u} - 216(14)e^{2}) \times 10^{-10} \\ &\delta_{G}a_{\mu}^{HVP,d/s} = (-1091(67)\Delta m_{d} - 13.5(9)e^{2}) \times 10^{-10} \\ &\delta_{G}a_{\mu}^{HVP,c} = (-59.2(3)\Delta m_{c} - 3.119(13)e^{2}) \times 10^{-10} \end{split}$$

$$\begin{split} &\delta_{G}a_{\mu}^{HVP,u} = (-4591(288)\Delta m_{u} - 227(15)e^{2}) \times 10^{-10} \\ &\delta_{G}a_{\mu}^{HVP,d/s} = (-1148(72)\Delta m_{d} - 14.2(1.0)e^{2}) \times 10^{-10} \\ &\delta_{G}a_{\mu}^{HVP,c} = (-57.2(2)\Delta m_{c} - 3.295(14)e^{2}) \times 10^{-10} \end{split}$$

 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_{U} (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

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

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

Hopping operators:

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

Expansion of Dirac operator

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 pion correlator



Divergence of variance

Consider the quantity at positive flowtime

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

- ▶ In QCD simulations, both A(t,x) and its variance are finite in the $V \to +\infty$ and $a \to 0$ 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 $V \to \infty$ limit and a^{-2} in the $a \to 0$ limit.

See talk at Lattice2024: Alessandro Cotellucci, Error Scaling of Sea Quark Isospin-Breaking Effects, Hadronic and nuclear spectrum and interactions, 1 August 2024 11:50















Summary

Full QCD+QED simulations:

- Simulations run as well/bad as QCD ones. More expensive because of C* boundary conditions and RHMC for all quarks.
- 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.
- ► 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
- We are calculating isospin-breaking corrections to HVP contribution to muon g 2 on QCD+QED configurations.

RM123 method:

- Reaching the gauge noise for the sea-quark insertions is painful but can be done.
- 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...
- 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. $c_{sw}^{SU(3)} = 2.18859$ and $c_{sw}^{U(1)} = 1$, same volume and β , but different κ_q and α :

ensemble	lattice	β	α	κ_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	
$\delta m_q = m_q^{A3}$	$^{380} - m_q^{A400}$			-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)
- 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_{μ}^{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:

$$\begin{split} \delta \boldsymbol{\sigma}_{\mu,(1)}^{HVP} &= \left(\frac{\alpha}{\pi}\right)^2 \int dt \, (Z_V^{(0)})^2 \delta G^{\ell\ell}(t) \tilde{K}(t;m_{\mu}) \\ G^{\ell\ell}(t) &= G^{\ell\ell}(t)^{(0)} + \delta G^{\ell\ell}(t) = G^{\ell\ell}(t)^{(0)} + \sum_f \delta m_f \left. \frac{\partial G^{\ell\ell}(t)}{\partial m_f} \right|_{(0)} + \left. \frac{e^2}{2} \left. \frac{\partial^2 G^{\ell\ell}(t)}{\partial e^2} \right|_{(0)} \end{split}$$

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 $(e^2, \delta m_u, \dots, \delta m_c)$ fixed to $\delta \epsilon_i = \underbrace{\epsilon_i^{A380a07}}_{QCD+QED} - \underbrace{\epsilon_i^{A400a00}}_{IsoQCD}$

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

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



With $G^{c\ell}(t)$, if conserved current $V^{c}_{\mu}(x)$ 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 $\lambda_3, \lambda_8, \lambda_{15}$:

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

Taking derivatives:

$$\frac{\partial Z_{V_{\mathcal{R}}V_{l}}}{\partial \varepsilon_{i}} = \lim_{x_{0} \to \infty} \left[\frac{\partial G^{cl}}{\partial \varepsilon_{i}}(x_{0}) - G^{cl}(x_{0}) (G^{\ell\ell}(x_{0}))^{-1} \frac{\partial G^{\ell\ell}}{\partial \varepsilon_{i}}(x_{0}) \right] \cdot (G^{\ell\ell}(x_{0}))^{-1}$$

Total correction:

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

Using mass shifts:

$$\delta Z_{V_R V_l} = \begin{pmatrix} -0.00002(19) & 0.000260(95) & 0.00027(11) & 0.000147(76) \\ 0.000230(93) & -0.00008(16) & 0.00027(11) & 0.00094(38) \\ 0.000133(54) & 0.00027(11) & -0.00005(19) & 0.000054(22) \\ 0.00030(15) & 0.00038(15) & 0.000217(87) & -0.000259(62)/2 \end{pmatrix}$$

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

QCD only ensembles						QCD+QED ensembles					
up/down/strange quark							1.0 1.0 (u, 3), (v), (v), (v), (v), (v), (v), (v), (v	5 10		up down/bitrange Charm	
type	$a_{\mu}^{u/d/s}\times 10^{-10}$	am _V ^{u/d/s}	$a^c_\mu imes 10^{-10}$	am _V ^c	-	type	$a^u_\mu imes 10^{10}$	am _V	$a_{\mu}^{d/s} \times 10^{10}$	$am_V^{d/s}$	$a_{\mu}^{c}\times 10^{10}$
Ensemble A400a00b324					-	Ensem	ble A380a07b	324, $\alpha_R = 0$.007		
11	338(8)	0.2644(50)	7.83(8)	0.8463(5)		11	-	-	-	-	-
cl	334(9)	0.2652(55)	6.18(7)	0.8462(5)		cl	331(7)	0.266(4)	83(2)	0.265(6)	9.78(10)
Ensemble B400a00b324					_	сс	-	-	-	-	-
11	// 402(9) 0.2522(33) 7.81(9) 0.8458(9)					Ensemble A360a50b324, $\alpha_R = 0.040633(80)$					
cl	397(9)	0.2530(32)	6.16(7)	0.8454(8)		cl	309(11)	0.267(8)	77(2)	0.262(7)	10.62(11)

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