HVP with C^{*} boundary conditions from lattice QCD(+QED)

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May 30, 2023

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1. Motivation

2. C* boundary conditions * Implementation

 \star RC^{*} ensembles

3. Methods for HVP and status of the work

- \star Results for QCD
- * Isospin breaking effects
- \star Results for QCD+QED

Motivation



- new results from the muon g-2 experiment expected soon
- lattice results for the window are in good agreement and in tension with R-ratio

Motivation

Isospin symmetry is violated at the percent level

- strong IBE $\sim \mathcal{O}((m_d m_u)/\Lambda_{QCD})$
- QED effects $\sim \mathcal{O}(\alpha_{EM})$

IBE effects are important for high-precision calculations of *decay rates of mesons*, *HVP contribution to g-2, etc.*

Theoretical issue of including QED in a finite periodic box:

- classical picture: Gauss law forbids a net non-zero charge
- path-integral: charged particles' propagation is forbidden due to symmetry under large gauge transformations

Currently used prescriptions for including QED:

- non-local constraints to remove the zero-modes of the photon [Hayakawa & Uno, 0804.2044] e.g QED_L, where $\sum_{\vec{x}} A_{\mu}(x_0, \vec{x}) = 0$
- infrared regulator m_γ (QED_M) [Endres et al., 1507.08916]
- QED_{∞} [Blum et al., 1705.01067; Feng & Jin, 1812.09817]
- QED_C [Kronfeld & Wiese, 1991, 1992; Polley, 1993; Lucini et al., 1509.01636]

• ...

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Local prescription for QED in a finite box \rightarrow C-periodicity of fields in spatial directions

$$\begin{aligned} A_{\mu}(x+L_{i}\hat{i}) &= -A_{\mu}(x) \qquad U_{\mu}(x+L_{i}\hat{i}) &= U_{\mu}^{*}(x) \\ \psi(x+L_{i}\hat{i}) &= C^{-1}\overline{\psi}(x) \qquad \overline{\psi}(x+L_{i}\hat{i}) &= -\psi^{T}(x)C \end{aligned}$$

 $[+] A_{\mu}(x) \text{ is C-odd} \implies p_i = \frac{\pi}{L_i}(2l_i + 1), \quad l_i = 0, 1, ..., L_i - 1$

[+] charged-states propagation is possible

[+] suppressed finite-volume effects [Lucini et al., 1509.01636 ; Martins & Patella, 2212.09565]

[-] violations of flavour and charge conservation (by boundary effects)

[-] more expensive simulations [Bushnaq et al., 2209.13183]

• Action in the doublet formulation

$$S_{F}^{hop} = -\frac{1}{2} \sum_{x \in \Lambda_{phys}, \mu} \overline{\chi}(x) \frac{(1+\gamma_{\mu})}{2} \mathbb{V}_{\mu}^{\dagger}(x-\mu) \chi(x-\hat{\mu}) + \overline{\chi}(x) \frac{(1-\gamma_{\mu})}{2} \mathbb{V}_{\mu}(x) \chi(x+\hat{\mu})$$

with

$$\chi(x) \equiv \begin{pmatrix} \psi(x) \\ \psi^{\mathcal{C}}(x) \end{pmatrix} \qquad \mathbb{V}_{\mu}(x) \equiv \begin{pmatrix} U_{\mu}(x)e^{iqA_{\mu}(x)} & 0 \\ 0 & U_{\mu}^{*}(x)e^{-iqA_{\mu}(x)} \end{pmatrix}$$

• Fields and their charge-conjugates associated with different space-time points

$$S_{F}^{hop} = -\frac{1}{2} \sum_{x \in \Lambda_{ext}, \mu} \overline{\psi}(x) \frac{(1+\gamma_{\mu})}{2} V_{\mu}^{\dagger}(x-\mu) \psi(x-\mu) + \overline{\psi}(x) \frac{(1-\gamma_{\mu})}{2} V_{\mu}(x) \psi(x+\mu)$$

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with

$$\chi(x) \equiv \begin{pmatrix} \psi(x) \\ \psi^{\mathcal{C}}(x) \end{pmatrix} \qquad \mathbb{V}_{\mu}(x) \equiv \begin{pmatrix} U_{\mu}(x)e^{iqA_{\mu}(x)} & 0 \\ 0 & U_{\mu}^{*}(x)e^{-iqA_{\mu}(x)} \end{pmatrix}$$

• Fields and their charge-conjugates associated with different space-time points

$$S_{F}^{hop} = -\frac{1}{2} \sum_{\mathbf{x} \in \Lambda_{ext}, \mu} \overline{\psi}(\mathbf{x}) \frac{(1+\gamma_{\mu})}{2} V_{\mu}^{\dagger}(\mathbf{x}-\mu) \psi(\mathbf{x}-\mu) + \overline{\psi}(\mathbf{x}) \frac{(1-\gamma_{\mu})}{2} V_{\mu}(\mathbf{x}) \psi(\mathbf{x}+\mu)$$

C* boundary conditions



- Lattice is doubled in direction $\hat{1}$: $L_1 = 2L$, $L_k = L$, k = 2, 3
- Orbifold construction, e.g $\psi(x + L_k \hat{k}) = \psi(x + \frac{L_1}{2}\hat{1})$
- Effective periodicity of 2L

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RC* collaboration's program

Seven ensembles generated thus far with the openQ*D code https://gitlab.com/rcstar/openQxD

First results in Bushnaq et al., 2209.13183

- details about the simulations
- calculations of meson masses, the Ω^- baryon, and the octet baryons
- cost analysis

Our setup allows for two ways of including isospin breaking effects:

- non-isosymmetric configurations at several unphysical values of α_{EM} and $m_u m_d$ + extrapolation to the physical point
- isosymmetric configurations with C^{\star} b.c. + RM123 method

QCD+QED ensembles

- Lüscher-Weisz SU(3) gauge action ($\beta = 3.24$)
- Wilson action for compact U(1) field
- $N_f = 1 + 2 + 1$ of O(a)-improved Wilson fermions
- Periodic boundary conditions in time, C* b.c. in space



- Volume: A=64x32, B=80x48, C=96x48
- $\bullet\,$ Lattice spacing $\simeq 0.05$ fm
- Pion mass between 360 and 500 MeV
- $m_\pi L \sim 3$ and $m_\pi L \sim 5$

QCD+QED ensembles

• Renormalization scheme ¹: $(8t_0)^{1/2}$, $\alpha_R(t_0)$, ϕ_0 , ϕ_1 , ϕ_2 , ϕ_3

$$\begin{split} \phi_0 &= 8t_0(m_{K^{\pm}}^2 - m_{\pi^{\pm}}^2) &\to 0 \quad (\text{fixes } m_s - m_d) \quad [\phi_0^{\text{phys}} = 0.992] \\ \phi_1 &= 8t_0(m_{K^{\pm}}^2 + m_{\pi^{\pm}}^2 + m_{K^0}^2) \to 2.11 \quad (\text{fixes } m_s + m_d + m_u) \quad [\phi_1^{\text{phys}} = 2.26] \\ \phi_2 &= 8t_0(m_{K^0}^2 - m_{K^{\pm}}^2)/\alpha_R &\to 2.36 \quad (\text{fixes } \delta m_{strong}/\delta_{EM}) \quad [\phi_2^{\text{phys}} = 2.36] \\ \phi_3 &= \sqrt{8t_0}(m_{D_5^{\pm}}^2 + m_{D^{\pm}}^2 + m_{D^0}^2) \to 12.1 \quad (\text{fixes } m_c) \quad [\phi_3^{\text{phys}} = 12.0] \end{split}$$

ensemble	V	flavor	β	α
A400a00b324	$64 imes 32^3$	3 + 1	3.24	0
B400a00b324	$80 imes 48^3$	3 + 1	3.24	0
A450a07b324	$64 imes 32^3$	1 + 2 + 1	3.24	0.007299
A380a07b324	$64 imes 32^3$	1 + 2 + 1	3.24	0.007299
A500a50b324	$64 imes 32^3$	1 + 2 + 1	3.24	0.05
A360a50b324	$64 imes 32^3$	1 + 2 + 1	3.24	0.05
C380a50b324	$96 imes 48^3$	1 + 2 + 1	3.24	0.05



 1 we used the CLS \textit{N}_{f} = 2 + 1 value of $\sqrt{\textit{8t}_{0}}$ = 0.415 fm [Bruno et al., 1608.08900]

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ensemble	V	flavor	α	<i>a</i> [fm] ²	$m_{\pi^\pm}[MeV]$
A400a00b324	$64 imes 32^3$	3 + 1	0	0.05393(24)	398.5(4.7)
B400a00b324	$80 imes 48^3$	3 + 1	0	0.05400(14)	401.9(1.4)
A450a07b324	$64 imes 32^3$	1 + 2 + 1	0.007299	0.05469(32)	451.2(4.3)
A380a07b324	$64 imes 32^3$	1 + 2 + 1	0.007299	0.05323(28)	383.6(4.4)
A500a50b324	$64 imes 32^3$	1 + 2 + 1	0.05	0.05257(14)	495.0(2.8)
A360a50b324	$64 imes 32^3$	1 + 2 + 1	0.05	0.05054(27)	358.6(3.7)
C380a50b324	$96 imes 48^3$	1 + 2 + 1	0.05	0.050625(79)	386.5(2.4)

- Reported measurements performed on 4 ensembles
- Ref: Altherr et al., 2212.11551, 2301.04385

 $^{^2}$ a is determined using the $N_f = 2 + 1$ value of $\sqrt{8t_0} = 0.415$ fm from Bruno et al., 1608.08900

HVP calculation

• Time-momentum representation

$$\begin{split} G(t) &= -\frac{1}{3} \sum_{k=1,2,3} \sum_{\vec{x}} \left\langle V_k^{c,l}(x) V_k^l(0) \right. \\ s_\mu^{HVP} &= \left(\frac{\alpha}{\pi}\right)^2 \sum_t G(t) \tilde{K}(t;m_\mu) \end{split}$$

• Two discretizations of the vector current

$$\begin{split} \mu' \\ V'_{\mu}(x) &= \sum_{f} q_{f} \overline{\psi}_{f}(x) \gamma_{\mu} \psi_{f}(x) \\ V^{c}_{\mu}(x) &= \sum_{f} \frac{1}{2} q_{f} \Big[\overline{\psi}_{f}(x+\hat{\mu}) \left(1+\gamma_{\mu}\right) U^{\dagger}_{\mu}(x) \psi_{f}(x) - \overline{\psi}_{f}(x) \left(1-\gamma_{\mu}\right) U_{\mu}(x) \psi_{f}(x+\hat{\mu}) \Big] \end{split}$$

• Extrapolation of the signal at large t (single-exponential for now)

 μ

HVP calculation

By considering the different Wick contractions:

$$\langle V_k^{\prime}(x)V_k^{\prime}(0)
angle = \sum_{f,f^{\prime}} q_f q_{f^{\prime}} \operatorname{tr} \left[\gamma_k D_f^{-1}(x|x)
ight] \cdot \operatorname{tr} \left[\gamma_k D_{f^{\prime}}^{-1}(0|0)
ight] +$$

 $-\sum_f q_f^2 \operatorname{tr} \left[\gamma_k D_f^{-1}(x|0) \gamma_k D_f^{-1}(0|x) \right]$

- $D_f^{-1}(x|y)$ quark propagator from y to x
- γ_k Dirac matrices (k = 1, 2, 3)

QCD configurations \rightarrow leading HVP (w/o IBE effects) QCD+QED configurations \rightarrow full HVP



ensemble	V	flavor	α	a[fm]	$m_{\pi^{\pm}}[MeV]$
A400a00b324	64×32^{3}	3 + 1	0	0.05393(24)	398.5(4.7)
B400a00b324	$80 imes 48^3$	3 + 1	0	0.05400(14)	401.9(1.4)
A450a07b324	64×32^{3}	1 + 2 + 1	0.007299	0.05469(32)	451.2(4.3)
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ensemble	V	β	α	$\kappa_{u,d,s}$	κ_c	c ^{SU(3)} SW
A400a00b324	$64 imes 32^3$	3.24	0	0.1344073	0.12784	2.18859
B400a00b324	$80 imes 48^3$	3.24	0	0.1344073	0.12784	2.18859

• Study of the signal-to-noise ratio for different discretizations of the correlator: G''(t), $G^{cl}(t)$, $G^{cc}(t)$



ensemble	V	β	α	$\kappa_{u,d,s}$	κ_c	c _{SW} (3)
A400a00b324	$64 imes 32^3$	3.24	0	0.1344073	0.12784	2.18859
B400a00b324	$80 imes 48^3$	3.24	0	0.1344073	0.12784	2.18859

• V^{I}_{μ} requires a renormalization constant and O(a)-improvement

 $V^{R}_{\mu,f}=Z^{m_f}_V(V^{I}_{\mu,f}+$ ac $_V\partial_
u au_{\mu
u,f})$ [Bhattacharya et al., 0511014]

 $egin{aligned} \mathcal{R}(t) = rac{\sum_{ec{x},k} \left\langle V_f^c(x) V_f'(0)
ight
angle}{\sum_{ec{x},k} \left\langle V_f'(x) V_f'(0)
ight
angle} \end{aligned}$

ensemble	$Z_V^{m_{l/s}}$	$Z_V^{m_c}$
A400a00b324	0.6745(12)	0.6066(2)
B400a00b324	0.6752(10)	0.6066(4)



QCD with C^* b.c.

 \bullet Connected LO-HVP for lattice volumes 64×32^3 and 80×48^3



ensemble	n. cnfg	type	am _V ^{u/d/s}	$a_{\mu}^{u/d/s} imes 10^{-10}$	am_V^c	$a^{c}_{\mu} imes 10^{-10}$
A400a00b324	200		0.2644(50)	338(8)	0.8463(5)	7.83(8)
		cl	0.2652(55)	334(9)	0.8462(5)	6.18(7)
B400a00b324	108		0.2522(33)	402(9)	0.8458(9)	7.81(9)
		cl	0.2530(32)	397(9)	0.8454(8)	6.16(7)

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Isosymmetric QCD configurations are generated with $m_u = m_d$, $\alpha_{em} = 0$

To include the strong and the QED ibe:

• perturbative expansion in $\alpha = e^2/4\pi$ and $\delta m = (m_d - m_u)/\Lambda_{QCD}$ [De Divitiis et al. 1303.4896]

$$\langle O(U, A, \psi, \bar{\psi}) \rangle_{QCD+QED} = \frac{1}{Z} \int \mathcal{D}U\mathcal{D}A \det[U, A] \exp(-S_g) \exp(-S_\gamma)O(U, A, \psi, \bar{\psi}) \langle V_{QCD+QED} \rangle + \frac{1}{Z} \int \mathcal{D}U\mathcal{D}A \det[U, A] \exp(-S_g) \exp(-S_\gamma)O(U, A, \psi, \bar{\psi}) \rangle$$

 $\rightarrow \det[U,A] \simeq \det[U] + \mathit{e_{sea}}det[U,A]' + \mathit{e_{sea}^2}det[U,A]''$

 $ightarrow {\cal O}_{QCD+QED} \simeq {\cal O}_{isoQCD} + \delta m {\cal O}_{\delta m}' + e_{val} {\cal O}_e' + e_{val}^2 {\cal O}_e''$

$$\begin{split} \left\langle V_k^{c,l}(x)V_k^l(0) \right\rangle &= \left\langle V_k^{c,l}(x)V_k^l(0) \right\rangle \bigg|_{e=0,m_f=\hat{m}} + \frac{1}{2}e^2 \frac{\partial^2}{\partial e^2} \left\langle V_k^{c,l}(x)V_k^l(0) \right\rangle \bigg|_{e=0,m_f=\hat{m}} + \\ &+ (m_f - \hat{m}) \frac{\partial}{\partial m_f} \left\langle V_k^{c,l}(x)V_k^l(0) \right\rangle \bigg|_{e=0,m_f=\hat{m}} + \dots \end{split}$$

[+] no need to generate new configurations

[+] corrections are measured as $\mathcal{O}(1)$ observables

[-] calculations of many diagrams needed

Photon propagator

• The photon field is Gaussian distributed in momentum space

$$S_{\gamma}^{Feyn.} = rac{1}{2} \sum_{k,\mu,
u} ilde{A}_{\mu}^{*}(k) \hat{k}_{
u}^{2} ilde{A}_{\mu}(k), \qquad \hat{k}_{\mu} = 2\sin{(rac{k_{\mu}}{2})}, \qquad k_{\mu} = rac{(2x_{\mu} + c_{\mu})\pi}{L_{\mu}}$$

• Propagator in the Feynman gauge is stochastically estimated with

$$\hat{A}_{\mu}(x) = rac{1}{\sqrt{N}} \sum_{k} rac{e^{-ikx}}{\sqrt{\hat{k}^2}} \tilde{B}_{\mu}(k), \qquad P(B) \propto \exp\left(-B_{\mu}^2(k)
ight)$$
 $\Lambda_{\mu
u}(x-y) = rac{\delta_{\mu
u}}{N} \sum_{k} rac{e^{ik(x-y)}}{\hat{k}^2} \simeq rac{1}{n_{src}} \sum_{i=1}^{n_{src}} \hat{A}^i_{\mu}(x) \hat{A}^i_{
u}(y)$

RM123 method

• Leading IB effects in the electro-quenched approximation $\implies e_{sea} = 0$



RM123 method

Work in progress...



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QCD+QED with C^{\star} b.c.

Simulation details:

ensemble	V	β	α	κ_u	$\kappa_{d,s}$	κ_c	$c_{SW}^{SU(3)}$	$c_{SW}^{U(1)}$
A380a07b324	$64 imes 32^3$	3.24	0.007299	0.13459164	0.13444333	0.12806355	2.18859	1
A360a50b324	$64 imes 32^3$	3.24	0.05	0.135560	0.134617	0.129583	2.18859	1

• Wilson action with compact U(1) field

$$S_{g,U(1)} = rac{1}{8\pi q_{el}^2 lpha} \sum_{x} \sum_{\mu \neq
u} [1 - P_{\mu
u}^{U(1)}(x)]$$

with q_{el} elementary charge, $P_{\mu\nu}^{U(1)}$ plaquette

- $c_{SW}^{SU(3)}$ correct up to $O(\alpha)$ terms, tree level improvement for U(1)
- $N_f = 1 + 2 + 1 \rightarrow \text{non-physical degenerate } d \text{ and } s \text{ quarks}$

QCD+QED with C^{\star} b.c.



Figure: Integrand of the connected HVP contribution for the A380a07b324 ensemble

- Results for the mixed correlator $G^{cl}(x_0)$
- Ren. constants are not considered yet

$$V^{ extsf{R}}_{\mu}(x) = V^{ extsf{c}}_{\mu}(x) + \mathcal{O}\left(\partial_{
u} \mathcal{F}^{
u\mu}
ight)$$
 [Collins et al., 0512187]

• signal-to-noise ratio similar to the QCD case

ensemble	n. cnfg	α_R	flavor	am_V	$a_{\mu}^{ m HVP} imes 10^{10}$
A360a50b324	181	0.040633(80)	up	0.267(8)	309(11)
			down/strange	0.262(7)	77(2)
			charm		10.62(11)
A380a07b324	200	0.007081(19)	up	0.266(4)	331(7)
			down/strange	0.265(6)	83(2)
			charm		9.78(10)

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- We computed the connected HVP on two QCD and two QCD+QED ensembles with C* b.c.
- Signal-to-noise ratio good for QCD and at the physical $\alpha_{\it EM}$
- The results are not extrapolated: a \sim 0.05, 360 $< m_\pi <$ 400 MeV
- Ongoing work:
 - \star RM123 method for QCD ensembles
 - \star disconnected diagrams for QCD and QCD+QED
 - * variance-reduction techinques: low-mode averaging [De Grand & Schaefer, 0401011]
- Long-term:
 - \star generation of new ensembles
 - $\star\,$ extrapolation to the physical point

Backup slides

- C^{*} boundaries in $\hat{i} \implies p_i = \frac{\pi}{L}(2\mathbb{Z}+1)$ for A_{μ}
- the vector current is a C-odd operator
- zero-momentum projection is not possible
- the spatial integration domain in TMR should be set to

$$\left(-\frac{L}{2},\frac{L}{2}\right)^3$$



Vector current in the doublet formulation

$$V_{\mu}^{loc}(x) := -\chi^{T}(x) \mathcal{K} C \frac{\gamma_{\mu}}{2} \tau_{3} \chi(x), \qquad \chi(x) \equiv \begin{pmatrix} \psi(x) \\ \psi^{C}(x) \end{pmatrix}, \quad \mathcal{K} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Vector current in the doublet formulation

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The (conn.) two-point functions has an extra Wick contraction

$$\chi(x)\chi(y) = -D^{-1}(x|y)KC^{-1}, \quad \left\langle \chi^{T}(x)KC\frac{\gamma_{\mu}}{2}\tau_{3}\chi(x)\chi^{T}(y)KC\frac{\gamma_{\nu}}{2}\tau_{3}\chi(y) \right\rangle$$

Vector current in the doublet formulation

$$V^{loc}_{\mu}(x) := -\chi^{T}(x) \mathcal{K}Crac{\gamma_{\mu}}{2} au_{3}\chi(x), \qquad \chi(x) \equiv \begin{pmatrix} \psi(x) \\ \psi^{\mathcal{C}}(x) \end{pmatrix}, \quad \mathcal{K} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad au_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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$$\chi(x)\chi(y) = -D^{-1}(x|y) \mathcal{K}C^{-1}, \quad \left\langle \chi^{\mathsf{T}}(x) \mathcal{K}C\frac{\gamma_{\mu}}{2} \tau_{3}\chi(x)\chi^{\mathsf{T}}(y) \mathcal{K}C\frac{\gamma_{\nu}}{2} \tau_{3}\chi(y) \right\rangle$$

In terms of Dirac spinors

$$\begin{split} &-\operatorname{tr}_{CD}[D^{-1}(x_1|y)\gamma_{\mu}\gamma_5 D^{-1\dagger}(x_1|y)\gamma_5\gamma_{\nu} - (D^{-1})(x_2|y)\gamma_{\mu}\gamma_5 (D^{-1})^{\dagger}(x_2|y)\gamma_5\gamma_{\nu}],\\ &\vec{x_1} \in (-L,L)^3, \qquad \vec{x_2} \in ((-2L,L) \cup (L,2L))^3 \end{split}$$

QCD with C^{*} b.c.: strange and charm contributions

 \bullet Connected LO-HVP for lattice volumes 64×32^3 and 80×48^3



ensemble	n. cnfg	type	am_V^s	$a_{\mu}^{s} imes 10^{-10}$	am_V^c	$a_{\mu}^{c} imes 10^{-10}$
A400a00b324	200		0.2808(22)	46.7(7)	0.8463(5)	7.83(8)
		cl	0.2796(29)	46.2(7)	0.8462(5)	6.18(7)
B400a00b324	108		0.2794(19)	48.5(7)	0.8458(9)	7.81(9)
		cl	0.2791(20)	48.0(7)	0.8454(8)	6.16(7)

QCD with C^{\star} b.c.: strange and charm contributions

• tuning of $\kappa_{s,c}^{\text{val}}$: change the valence hopping parameters such that $m_V^{s\bar{s}}$, $m_V^{c\bar{c}}$ match (disconnected and QED effects are neglected)

$$m_{\phi}^{phys}=1019.461(20){
m MeV}$$

 $m_{J/\psi}^{phys} = 3096.900(6) {
m MeV}$



QCD+QED with C^{\star} b.c.

• comparison of the relative error for three values of $\boldsymbol{\alpha}$



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