





Update on the RM123 method

Alessandro Cotellucci

ETH Zürich, January 29th 2024



Map

- 1 RM123: The Story So Far
 - 1.1 Method
 - 1.2 Sea-Sea diagrams
 - 1.3 Sea-Valence and Valence-Valence for mesons
- 2 The $N_f = 3$
- 3 What is next?

The method

The observable $\mathcal{O}[U, A, \chi]$ on the full path integral^a:

$$\begin{split} \langle \mathcal{O} \rangle &= \frac{\int dU d\chi dA \ e^{-S_{\rm Iso}[U,\chi]} e^{-S_{\rm IB}[U,A,\chi]} e^{-S_{\gamma}[A]} \mathcal{O}[U,A,\chi]}{\int dU d\chi dA \ e^{-S_{\rm Iso}[U,\chi]} e^{-S_{\rm IB}[A,\chi,U]} e^{-S_{\gamma}[A]}} \\ &= \frac{\langle \int dA \ e^{-S_{\rm IB}[U,A,\chi]} e^{-S_{\gamma}[A]} \mathcal{O}[U,A,\chi] \rangle_{\rm Iso}}{\langle \int dA \ e^{-S_{\rm IB}[U,A,\chi]} e^{-S_{\gamma}[A]} \rangle_{\rm Iso}} \\ &= \langle \mathcal{O} \rangle_{\rm Iso} - \langle \underbrace{S_{\rm IB} \mathcal{O}} \rangle_{\rm Iso\gamma,c} + \frac{1}{2} \langle \underbrace{S_{\rm IB} S_{\rm IB} \mathcal{O}} \rangle_{\rm Iso\gamma,c}}_{valence-valence}} + \underbrace{\langle \overset{I}{S} \underset{\rm IB}{S} \overset{I}{S} \underset{\rm IB}{S} \mathcal{O}} \rangle_{\rm Iso\gamma,c}}_{sea-sea} \\ &+ o \left(\delta m_{ud}^2, e^4, e^2 \delta m_{ud} \right). \end{split}$$

^aDivitiis et al., "Leading isospin breaking effects on the lattice".

RM123: The Story So Far Sea-Sea Diagrams

Considering a pure gluonic observable $\ensuremath{\mathcal{O}}$ the disconnected terms are:

$$\begin{split} \langle \mathcal{O} \rangle = & \langle \mathcal{O} \rangle_{\rm Iso} - \delta \beta \langle S_{gauge} \mathcal{O} \rangle_{\rm Iso,c} + \sum_{f} \delta m_{f} \langle \bigodot^{\rm f} \mathcal{O} \rangle_{\rm Iso,c} \\ & + e^{2} \left[\sum_{f} \hat{q}_{f}^{2} \left(\langle \bigodot^{\rm f}_{\rm Los} \mathcal{O} \rangle_{\rm Iso,c} + \langle \underbrace{\stackrel{\rm f}{\textcircled{}}}_{\rm Los} \mathcal{O} \rangle_{\rm Iso,c} \right) \\ & + \sum_{fg} \hat{q}_{f} \hat{q}_{g} \langle \overset{\rm f}{\bigcirc}_{\rm Los} \overset{\rm g}{\bigcirc} \mathcal{O} \rangle_{\rm Iso,c} \right]. \end{split}$$

Sea-Sea Diagrams

Sea-Sea Diagrams: Results

lattice	<i>a</i> [fm]	m_{π} [MeV]	m_D [MeV]	no. cnfg	nsrc per lv per cnfg
$64 imes 32^3$	0.05393(24)	398.5(4.7)	1912.7(5.7)	50	400
$80 imes 48^3$	0.05400(14)	401.9(1.4)	1908.5(4.5)	50	100

Table: Configurations used^b.

Parameters used:

$$\delta \beta = \delta c_{SW}^{SU(3)f} = 0$$

$$c_{SW}^{U(1)f} = 1$$

$$e = e_{phys}$$

$$\delta m_f \text{ from QCD+QED simulation.}$$

From QCD $N_f = 3 + 1$ to QCD+QED $N_f = 1 + 2 + 1$.

^bBushnaq et al., "First results on QCD+QED with C* boundary conditions".

Sea-Sea Diagrams: to

The scale is set using the auxiliary Wilson-flow observable t_0 :

$$t_0^2 \langle E(t) \rangle \big|_{t=t_0} = 0.3$$

Observable	Value [lattice units]
t_0^{QCD}	7.36 ± 0.04
δt_0^{Mass}	$\textbf{0.28} \pm \textbf{0.21}$
δt_0^{Tad}	-0.49 ± 0.27
$\delta t_0^{\text{Bubbles}}$	-0.01 ± 0.06
δt_0^{Self}	0.12 ± 0.13
δt_0^{Tot}	-0.11 ± 0.13
$t_0^{\text{QCD}+\text{QED}_{\text{RM123}}}$	7.26 ± 0.14
$t_0^{\text{QCD}+\text{QED}}$	7.54 ± 0.05

Table: IBE effects on t_0 for A400a00b324.

Sea-Sea Diagrams: to error on A400a00b324



Sea-sea IBE effect to t₀/a² for A400a00b324

Sea-Sea Diagrams: to error on B400a00b324



Sea-sea IBE effect to t₀/a² for B400a00b324

Sea-Sea Diagrams: Volume scaling of the variance

For a gluonic quantity like E(t) the scaling of the error is $a^{-1}\sqrt{V}$ for strong isospin-breaking effects and $a^{/2}\sqrt{V}$ for electro-magnetic isospin-breaking effects.



Scaling of the error for light quarks

Sea-Sea Diagrams: Volume scaling of the variance



Scaling of the error for charm quark

Sea-Sea Diagrams: $m_{\pi^{\pm}}$

Sea-sea contribution to the pion mass.

Observable	Value [MeV]
$m_{\pi^{\pm}}^{ extsf{QCD}}$	408 ± 7
$\delta m_{\pi^\pm}^{\sf Mass}$	-63 ± 41
$\delta m_{\pi^\pm}^{\sf Tad}$	50 ± 60
$\delta m_{\pi^{\pm}}^{Bubbles}$	7 ± 9
$\delta m^{Self}_{\pi^\pm}$	-27 ± 25
$\delta m_{\pi^\pm}^{\sf Tot}$	-32 ± 20
$m_{\pi^{\pm}}^{ extsf{QCD}+ extsf{QED}_{ extsf{RM123}}}$	375 ± 21
$m_{\pi^{\pm}}^{ extsf{QCD+QED}}$	401 ± 7

Table: Sea-Sea IBE effects on $m_{\pi^{\pm}}$ on A400a00b324.

Sea-Sea Diagrams: $m_{\pi^{\pm}}$ error on A400a00b324



Sea-sea IBE effect to mn[±] for A400a00b324

Sea-Sea Diagrams: $m_{\pi^{\pm}}$ error on B400a00b324



Sea-sea IBE effect to mn[±] for B400a00b324

Sea-Sea Diagrams: Achievements and Future Plan

Achievements:

- ✓ The gauge noise can be achieved for the sea-sea diagrams;
- ✓ The O(a) improvement term reach faster the gauge noise;
- ✓ The precision in the RM123 method is worse than the full simulations for the same number of gauge configurations;
 Future plan:
 - To compare stochastic and exact photon;
 - To study the scale of the error in $a o 0, \ V o \infty$ and $m_\pi o m_{\pi^{
 m phys.}}$;

Valence-Valence for mesons

$$\begin{split} \sum_{z} \operatorname{Re} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, z) D_{f}^{-1}(z, x) \right] = \underbrace{+}_{s} \\ \frac{1}{2} \sum_{zw} \langle \operatorname{Re} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, z) T(z, w) D_{f}^{-1}(w, x) \right] \rangle_{\gamma} = \underbrace{+}_{s} \\ - \sum_{zwlm} \langle \operatorname{Re} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, z) J(z, w) D_{f}^{-1}(w, l) J(l, m) D_{f}^{-1}(m, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{5}}{16} \sum_{zw} \langle \operatorname{Re} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, z) J(z, w) D_{f}^{-1}(z, w) \sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(w) D_{f}^{-1}(w, x) \right] \rangle_{\gamma} \\ \frac{c_{f}}{2} \sum_{zwk} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, z) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(z) D_{f}^{-1}(z, w) J(w, k) D_{f}^{-1}(k, x) \right] \rangle_{\gamma} \\ \frac{c_{f}}{2} \sum_{zwk} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, y) \gamma_{5} D_{f}^{-1}(y, w) J(w, z) D_{f}^{-1}(z, w) J(w, k) D_{f}^{-1}(k, x) \right] \rangle_{\gamma} \\ - \sum_{wwh} \langle \operatorname{Retr} \left[\gamma_{5} D_{s}^{-1}(x, l) J(l, m) D_{s}^{-1}(m, y) \gamma_{5} D_{f}^{-1}(y, w) J(w, z) D_{f}^{-1}(z, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{5}}{8} \sum_{zw} \langle \operatorname{Retr} \left[\gamma_{5} D_{s}^{-1}(x, l) J(l, m) D_{s}^{-1}(m, y) \gamma_{5} D_{f}^{-1}(y, w) J(w, z) D_{f}^{-1}(z, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{5}}{8} \sum_{zw} \langle \operatorname{Retr} \left[\gamma_{5} D_{s}^{-1}(x, z) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(z) D_{s}^{-1}(z, y) \gamma_{5} D_{f}^{-1}(y, w) \sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(w) D_{f}^{-1}(w, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{5}}{2} \sum_{zwk} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, z) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(z) D_{s}^{-1}(z, y) \gamma_{5} D_{f}^{-1}(y, w) \sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(w) D_{f}^{-1}(w, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{5}}{2} \sum_{zwk} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, z) J(z, w) D_{s}^{-1}(w, y) \gamma_{5} D_{f}^{-1}(y, k) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(k) D_{f}^{-1}(k, x) \right] \rangle_{\gamma} \\ \frac{c_{f} c_{2}}{2} \sum_{zwk} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_{5} D_{s}^{-1}(x, z) J(z, w) D_{s}^{-1}(w, y) \gamma_{5} D_{f}^{-1}(y, k) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(k) D_{f}^{-1}(k, x) \right] \rangle_{\gamma} \\ 14/23 \end{aligned}$$

Valence-Valence: Mass and Tadpole on A400a00b324

Valence IBE to the K⁰ effective mass [Lattice units]



Figure: Valence-Valence IBE correction to the effective mass m_{K^0} (only from the mass and tadpole) with 30 random sources [Preliminary].

Valence-Valence on A400a00b324

Looking at what Paola already computed for m_{K^0} we have:

$$\delta am_{K^0} = (\delta am_d + \delta am_s)4.7(2) + e^20.22(1)$$

Compatible inside of 2σ .

Sea-Valence for mesons

The Sea-Valence effects to compute are:

$$- \frac{1}{4} \sum_{zwkl} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_5 D_s^{-1}(x, y) \gamma_5 D_f^{-1}(y, z) J(z, w) D_f^{-1}(w, x) \right] \operatorname{Im} \operatorname{tr} \left[J(k, l) D_g^{-1}(l, k) \right] \rangle_{\gamma}$$

$$- \frac{c_g c_f}{64} \sum_{\substack{zw \\ \mu\nu\rho\sigma}} \langle \operatorname{Re} \operatorname{tr} \left[\gamma_5 D_s^{-1}(x, y) \gamma_5 D_f^{-1}(y, z) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(z) D_f^{-1}(z, x) \right] \operatorname{Re} \operatorname{tr} \left[\sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(w) D_g^{-1}(w, w) \right] \rangle_{\gamma}$$

$$- \frac{c_g}{16} \sum_{\substack{zwk \\ \mu\nu}} \langle \operatorname{Im} \operatorname{tr} \left[\gamma_5 D_s^{-1}(x, y) \gamma_5 D_f^{-1}(y, z) J(z, w) D_f^{-1}(w, x) \right] \operatorname{Re} \operatorname{tr} \left[\sigma_{\mu\nu} \hat{A}_{\mu\nu}(k) D_g^{-1}(k, k) \right] \rangle_{\gamma}$$

$$- \frac{c_f}{16} \sum_{\substack{zwk \\ \mu\nu}} \langle \operatorname{Re} \operatorname{tr} \left[\gamma_5 D_s^{-1}(x, y) \gamma_5 D_f^{-1}(y, z) \sigma_{\mu\nu} \hat{A}_{\mu\nu}(z) D_f^{-1}(z, x) \right] \operatorname{Im} \operatorname{tr} \left[J(w, k) D_g^{-1}(k, w) \right] \rangle_{\gamma}$$



Sea-Valence: Noise problem

Sea-valence IBE to the K⁰ effective mass [Lattice units]



Figure: Sea-Valence IBE correction to the effective mass m_{K^0} (only from the current) with 30 random sources on A400a00b324 [Preliminary].

Sea-Valence and Valence-Valence Diagrams: Plans

Plans:

- Strict test with numerical derivatives;
- Use the analytic photon for the sea-valence to recycle the sea-sea bubble;
- Extend to the complete ensembles A400a00b324 and B400a00b324;

 $N_f = 3$ Project

New Ensembles

We plan to generate the following ensembles:

ensemble	lattice	β	$c_{\rm sw}$	n.cnfg.	$\kappa_{u,d,s}$	M_{π} [MeV]	a [fm]	$M_{\pi}L$
C420a00b370	64×32^{3}	3.70	1.70477	2000	0.137	420	0.049	3.3
B420a00b346	48×24^3	3.46	1.915595	2000	0.13689	420	0.075	3.8
D270a00b346	96×48^3	3.46	1.915595	500	0.136994	270	0.075	4.9
A420a00b334	32×16^3	3.34	2.066858	2000	0.1365716	420	0.098	3.3
B420a00b334	48×24^3	3.34	2.066858	2000	0.1365716	420	0.098	5.0
C420a00b334	64×32^3	3.34	2.066858	2000	0.1365716	420	0.098	6.7

Table: $N_f = 3$ ensembles that we plan to generate in the project, for all the ensembles we will use CLS tuned parameters^c.

 $[^]c\mbox{Bali}$ et al., "Scale setting and the light baryon spectrum in $N_f=2+1$ QCD with Wilson fermions".

$N_f = 3$ Project

New Ensembles



The steps of the project are:

- To generate of $N_f = 3$ with different *a*, *V*, m_{π} ;
- To measure sea-sea, sea-valence and valence valence diagrams.

The main objective is to study the scaling of the sea-sea, sea-valence and valence-valence contributions in the limits $a \to 0$, $V \to \infty$ and $m_{\pi} \to m_{\pi}^{\text{phys.}}$.

What is next?

- Can these configurations be useful for HVP, Baryons and other observables?
- What is the effect of these sea-sea diagrams on other observables?

Thank you for your attention!

Acknowledgments

The work was supported by the North-German Supercomputing Alliance (HLRN) with the project bep00102 and bep00116.

References I

- [1] Gunnar S. Bali et al. "Scale setting and the light baryon spectrum in $N_f = 2 + 1$ QCD with Wilson fermions". In: JHEP 05 (2023), p. 035. DOI: 10.1007/JHEP05(2023)035. arXiv: 2211.03744 [hep-lat].
- [2] Lucius Bushnaq et al. "First results on QCD+QED with C* boundary conditions". In: JHEP 03 (2023), p. 012. DOI: 10.1007/JHEP03(2023)012. arXiv: 2209.13183 [hep-lat].
- G. M. de Divitiis et al. "Leading isospin breaking effects on the lattice". In: *Phys. Rev. D* 87 (11 2013), p. 114505. DOI: 10.1103/PhysRevD.87.114505. URL: https: //link.aps.org/doi/10.1103/PhysRevD.87.114505.

Backup Mass Term Estimator

The mass term has been estimated using the following method:

$$\text{Tr} \left[D_{m_u}^{-1} \right] \sim \left(m_c - m_u \right) \frac{1}{N_s} \sum_{i}^{N_s} \left(D_{m_c}^{\dagger} \eta_i \right)^{\dagger} D_{m_u} \eta_i \\ + \sum_{i}^{N_{pr}} s_i^{\dagger} S W^{-1} \sum_{n=0}^{3} \left(-HSW^{-1} \right)^n s_i \\ + \frac{1}{N_s} \sum_{i}^{N_s} \xi_i^{\dagger} \left(-SW^{-1} H \right)^4 D_{m_c}^{-1} \xi_i$$

Backup Tadpole Term Estimator

-

The tadpole term has been estimated using the following method:

$$\operatorname{Tr}\left[TD_{m_{u}}^{-1}\right] \sim (m_{c} - m_{u}) \frac{1}{N_{s}} \sum_{i}^{N_{s}} \left(D_{m_{c}}^{\dagger} \eta_{i}\right)^{\dagger} TD_{m_{u}} \eta_{i}$$
$$+ \sum_{i}^{N_{pr}} s_{i}^{\dagger} TSW^{-1} \sum_{n=0}^{2} \left(-HSW^{-1}\right)^{n} s_{i}$$
$$+ \frac{1}{N_{s}} \sum_{i}^{N_{s}} \xi_{i}^{\dagger} T \left(-SW^{-1}H\right)^{3} D_{m_{c}}^{-1} \xi_{i}$$

Backup

Bubbles Estimator

Due to SU(3) flavour symmetry, the only bubbles contributing are the charm bubbles:

$$\begin{bmatrix} JD_{m_{c}}^{-1} \end{bmatrix}_{i}^{a} = \sum_{j}^{N_{pr}} s_{j}^{\dagger} J^{a} SW^{-1} \sum_{n=0}^{2} (-HSW^{-1})^{n} s_{j} + \xi_{i}^{\dagger} J^{a} (-SW^{-1}H)^{3} D_{m_{c}}^{-1} \xi_{i} \begin{bmatrix} \sigma_{\mu\nu} \hat{A}_{\mu\nu} D_{m_{c}}^{-1} \end{bmatrix}_{i}^{a} = \sum_{j}^{N_{pr}} s_{j}^{\dagger} \sigma_{\mu\nu} \hat{A}_{\mu\nu}^{a} SW^{-1} \sum_{n=0}^{3} (-HSW^{-1})^{n} s_{j} + \xi_{i}^{\dagger} \sigma_{\mu\nu} \hat{A}_{\mu\nu}^{a} (-SW^{-1}H)^{4} D_{m_{c}}^{-1} \xi_{i}$$

The stochastic estimator will be:

$$\operatorname{Tr}\left[JD_{m_{c}}^{-1}\right]\operatorname{Tr}\left[JD_{m_{c}}^{-1}\right] \sim \frac{2}{N_{s}\left(N_{s}-1\right)}\sum_{i\neq j}^{N_{s}}\frac{1}{N_{A}}\sum_{a}^{N_{A}}\left[JD_{m_{c}}^{-1}\right]_{i}^{a}\left[JD_{m_{c}}^{-1}\right]_{j}^{a}$$

Backup Self-Energy Estimator

The tadpole term has been estimated using the following method:

$$\mathsf{Tr} \left[J D_{m_u}^{-1} J D_{m_u}^{-1} \right] \sim (m_c - m_u) \frac{1}{N_s} \sum_{i}^{N_s} \left(D_{m_c}^{\dagger} \eta_i \right)^{\dagger} J D_{m_u}^{-1} J D_{m_u} \eta_i \\ + \frac{1}{N_s} \sum_{i}^{N_s} \xi_i^{\dagger} J D_{m_u}^{-1} J D_{m_c}^{-1} \xi_i$$

Valence-Valence Diagrams: m_{K^0}

Observable	Value [MeV]
$m_{\kappa^0}^{\text{QCD}}$	408 ± 7
$\delta m_{K^0}^{Mass}$	-26 ± 1
$\delta m_{K^0}^{Tad}$	69 ± 5
$\delta m_{K^0}^{\text{Self}}$	-18 ± 1
$\delta m_{K^0}^{Exch.}$	$\textbf{0.54} \pm \textbf{0.06}$
$\delta m_{\kappa^0}^{\text{Angl.}}$	37 ± 19
$\delta m_{K^0}^{\text{Tot}}$	62 ± 20
$m_{K^0}^{\text{QCD}+\text{QED}_{\text{RM123}}}$	470 ± 22
$m_{K^0}^{\text{QCD}+\text{QED}}$	405 ± 8

Valence-Valence contribution to the kaon mass.

Table: Valence-Valence IBE effects on m_{K^0} on A400a00b324.