Efficiently unquenching QCD+QED at $O(\alpha)$

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THE UNIVERSITY *of* EDINBURGH

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Unquenching at leading-order

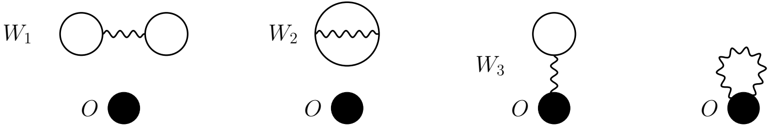
In QCD+QED it is practical to expand in the electric charge e

$$\langle O \rangle = \langle O \rangle \Big|_{e=0} + \frac{1}{2} e^2 \frac{\partial}{\partial e} \frac{\partial}{\partial e} \langle O \rangle \Big|_{e=0} + \dots$$

The leading corrections are determined by double insertions of the vertex

$$(-\mathrm{i})^2 \int_x J_\mu(x) A_\mu(x) \int_y J_\nu(y) A_\nu(y), \qquad J_\mu = \tfrac{2}{3} \bar{u} \gamma_\mu u - \tfrac{1}{3} \bar{d} \gamma_\mu d - \tfrac{1}{3} \bar{s} \gamma_\mu s,$$

which give rise to the Wick contractions



Omission of $W_{1,2,3}$ is equivalent to setting $e = 0$ in the fermion determinant

[1] G. M. de Divitiis, R. Frezzotti, V. Lubicz, et al. In: *Phys. Rev. D* 87.11 (2013), p. 114505.
[2] S. Borsanyi et al. In: *Nature* 593.7857 (2021), pp. 51–55.

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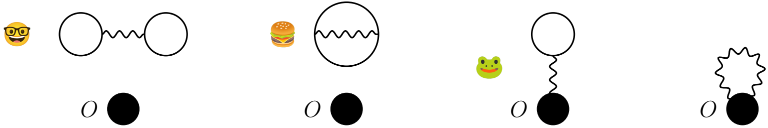

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Short-distance dominance in the variance

The leading corrections are defined by fully-connected correlators

$$\langle OW_1 \rangle_{\mathrm{conn}} = \langle OW_1 \rangle - \langle O \rangle \langle W_1 \rangle,$$

so that, in the Gaussian approximation, the variance factorizes

$$\sigma^2_{OW_1} \approx \sigma^2_O \sigma^2_{W_1} + \langle OW_1 \rangle^2_{\mathrm{conn}} \approx \sigma^2_O \sigma^2_{W_1}.$$

Therefore it's useful to analyse the variance of $W_{1,2}$

$$\sigma^2_{W_{1,2}} = \langle W^2_{1,2} \rangle - \langle W_{1,2} \rangle^2,$$

which has a contact term when all fields coincide

$$a^{12} L^4 \underbrace{J_\mu A_\mu J_\nu A_\nu J_\rho A_\rho J_\sigma A_\sigma}_{a^{-16}} \sim \frac{L^4}{a^4} \mathbb{I} + \ldots,$$

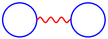
so is dominated by the short-distance contribution as $a \to 0$.

Translation averaging

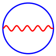
With translation averaging, short-distance contributions suppressed by $(a/L)^4$

Implement using stochastic estimators for the traces of quark propagators S

$$H_1(x,y) = \sum_{f,g} Q_f Q_g \,\mathrm{tr}\left\{\gamma_\mu S^f(x,x)\right\} \mathrm{tr}\left\{\gamma_\mu S^g(y,y)\right\},$$

W_1 

$$H_2(x,y) = -\sum_f Q_f^2 \,\mathrm{tr}\left\{\gamma_\mu S^f(x,y)\gamma_\mu S^f(y,x)\right\}$$

W_2 

which determine $W_{1,2}$ by the convolution with photon propagator G

$$W_{1,2} = -a^8 \sum_{x,y} H_{1,2}(x,y) G(x-y).$$

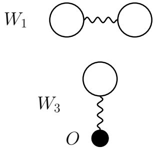
$\rightsquigarrow$ avoid stochastic sampling of Maxwell action

Single-propagator trace

W_1 and W_3 contain the single traces

$$\sum_{f=\mathrm{u,d,s}} Q_f \mathrm{tr}\{\gamma_\mu S^f\} = \frac{1}{3}\mathrm{tr}\{\gamma_\mu (S^{\mathrm{ud}} - S^{\mathrm{s}})\}$$

if $m_{\mathrm{u}} = m_{\mathrm{d}}$ when $e = 0$



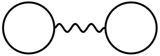
Using identity $S^{\mathrm{ud}} - S^{\mathrm{s}} = (m^{\mathrm{s}} - m^{\mathrm{ud}}) S^{\mathrm{ud}} S^{\mathrm{s}}$

- the trace is suppressed by $m^{\mathrm{s}} - m^{\mathrm{ud}}$
- the variance is finite $a^{-4} \to (m^{\mathrm{s}} - m^{\mathrm{ud}})^4$
- an efficient *split-even* estimator is known for the trace (cf. one-end trick for TM)

$$\mathcal{T}_i(x) = \tfrac{1}{3}(m^{\mathrm{s}} - m^{\mathrm{ud}})\{\eta_i^\dagger S^{\mathrm{ud}}\}(x)\gamma_\mu\{S^{\mathrm{s}}\eta_i\}(x).$$

[3] L. Giusti et al. In: *Eur. Phys. J. C* 79.7 (2019), p. 586.
[4] P. Boucaud et al. In: *Comput. Phys. Commun.* 179 (2008), pp. 695–715.

W_1 quark–line disconnected



The W_1 contraction can be estimated as

$$\mathcal{W}_1 \approx \frac{1}{N_\mathrm{s}(N_\mathrm{s}-1)} \sum_{i \neq j} \left(a^4 \sum_x \mathcal{T}_i(x) \right) \left(a^4 \sum_y \mathcal{T}_j(y) G(x-y) \right)$$

where the convolution $\sum_y \mathcal{T}_j(y) G(x-y)$ can be computed efficiently with the FFT

Leading extra contribution to variance scales like $1/N_\mathrm{s}^2$

$$\sigma^2_{\mathcal{W}_1} = \sigma^2_{W_1} + \frac{1}{N_\mathrm{s}^2} \# + \dots$$

Numerical set-up

L/a	T/a	m_π	$m_\pi L$	a	$N_{\rm cfg}$
24	64	340 MeV	4.9	0.12 fm	50

Table: C1 Ensemble

QCD configurations generated by the RBC/UKQCD configuration

- $N_{\rm f} = 2 + 1$ domain-wall fermions $\rightsquigarrow$ chiral regularization
- local discretization of the current (no new divergences)

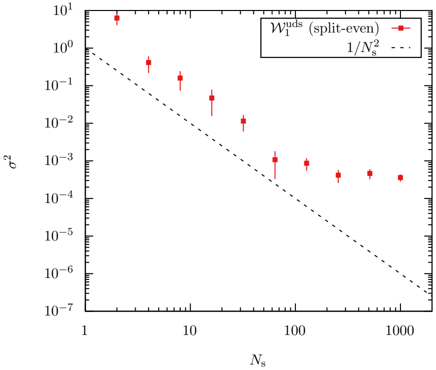
In the following we use $\mathrm{QED_L}$ in Feynman gauge

$$\widetilde{G}(\hat{k}) = \frac{1}{\hat{k}^2} \quad \text{and} \quad 0 \quad \text{when} \quad \hat{\boldsymbol{k}} = \mathbf{0}.$$

[5] T. Blum et al. In: *Phys. Rev. D* 93.7 (2016), p. 074505.

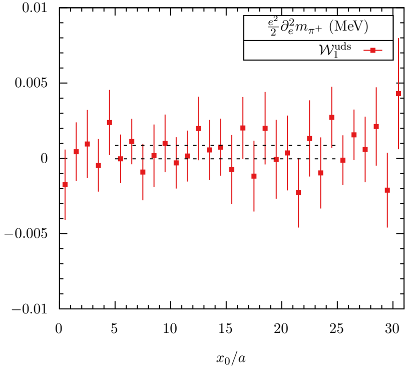
[6] M. Hayakawa and S. Uno. In: *Prog. Theor. Phys.* 120 (2008), pp. 413–441.

Numerical results W_1



- Scaling with N_s^{-2}
- Saturation of gauge variance with $N_s \sim \mathrm{O}(100)$ inversions

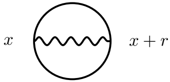
Numerical results W_1



Correction to charged pion mass due to W_1

$$\frac{e^2}{2}\partial_e^2 m_{\pi^+}^2 = 0.0004(0.0005)\ \mathrm{MeV}$$

W_2 quark-line connected



Naïve stochastic estimator

$$\mathcal{H}_2(x, x+r) = \sum_f Q_f^2 \frac{1}{N_s(N_s-1)} \sum_{i \neq j} \mathrm{tr}\{\gamma_\mu \Sigma_i^f(x, x+r) \gamma_\mu \Sigma_j^f(x+r, x)\},$$

$$\Sigma_i^f(x, x+r) = \{S^f \eta_i\}(x) \eta_i^\dagger(x+r)$$

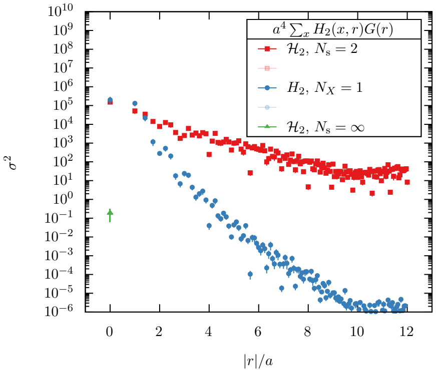
can be computed efficiently for small number of $r = x - y$

$\Rightarrow$ split estimator into $|r| \leq R$ and $|r| > R$ parts

$$\mathcal{W}_2 = a^8 \sum_{|r| \leq R} \sum_x \mathcal{H}_2(x, x+r) G(r) + a^4 \frac{L^4}{N_X} \sum_{\{X\}} \sum_{|r|>R} H_2(X, X+r) G(r)$$

[7] G. M. de Divitiis, R. Frezzotti, M. Masetti, et al. In: *Phys. Lett. B* 382 (1996), pp. 393–397.

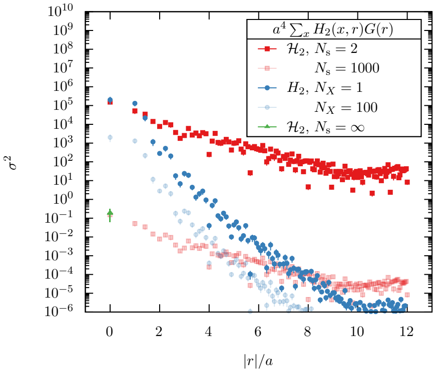
Numerical results W_2



Choose $R/a \sim 4$ reach full translation averaging with

- short-distance piece with $N_s \sim \mathrm{O}(1000)$ stochastic samples
- long-distance piece with $N_X \sim \mathrm{O}(100)$ point sources

Numerical results W_2



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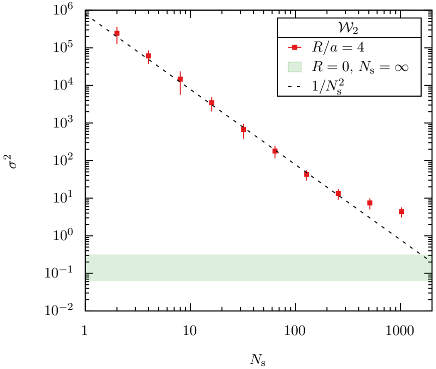

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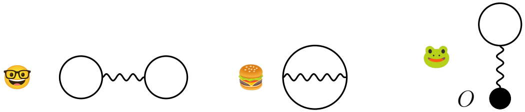
Conclusions



$W_{1,3}$ considering uds contribution + *split-even* estimator

- $\boxed{\frac{e^2}{2}\partial_e^2 m_{\pi^+}^2 = 0.0004(0.0005)\ \mathrm{MeV}}$

W_2 variance dominated by short distances $\sigma_{W_2}^2 \sim a^{-4}$

- split in to short- and long-distance parts
- full translation averaging can be achieved with moderate cost

$W_{1,2}$ diagrams can be reused for any observable ($g-2$, $K_{\ell 2}$, $\ldots$)

W_3 diagrams require inversions for each observable

Mass differences for domain-wall fermions

Recall the definition of $\tilde{D}$ in terms of the 5D Wilson matrix

$$\tilde{D}^{-1} = (\mathcal{P}^{-1} D_5^{-1} R_5 \mathcal{P})_{11}$$

from which the result is obtained immediately

$$\tilde{D}_r^{-1} - D_s^{-1} = (m^s - m^r)(\mathcal{P} D_{5,r}^{-1} R_5 D_{5,s}^{-1} R_5)_{11}$$

by noting that the following matrix projects on the physical domain

$$(R_5)_{\cdot\cdot} = (R_5 \mathcal{P})_{\cdot 1} (\mathcal{P}^{-1})_{1\cdot\cdot}$$

The preceding identity is easily demonstrated using the explicit representations

$$R_5 = \begin{pmatrix} & P^+ \\ P^- & \end{pmatrix}, \qquad \mathcal{P}^{-1} = \begin{pmatrix} P_- & & & P_+ \\ P_+ & & & \\ & \ddots & & \\ & & P_+ & P_- \end{pmatrix},$$

and $P_\pm = 1 \pm \gamma_5$.

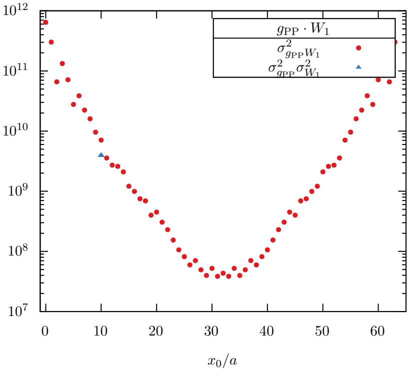
Factorization of the variance

Check of factorization of the variance

$$\sigma^2_{OW_1} \approx \sigma^2_O \sigma^2_{W_1},$$

for the connected correlator

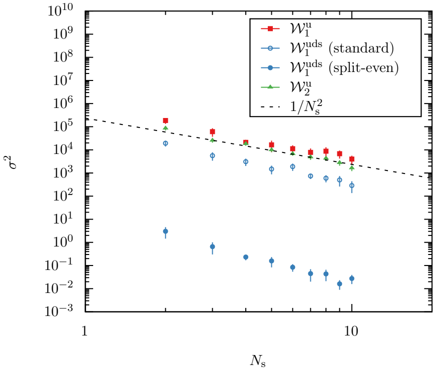
$$\langle OW_1 \rangle_{\text{conn.}} = \langle OW_1 \rangle - \langle O \rangle \langle W_1 \rangle, \qquad O \equiv g_{\text{PP}}(x_0) = a^3 \sum_{\boldsymbol{x}} P^{12}(x) P^{21}(0)$$



(no charge factors included, bare current)

Comparison of stochastic estimators

Comparison of stochastic estimators for W_1 and W_2



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