Efficient simulations with electrically-charged sea-quarks at $\mathrm{O}(\alpha)$

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Tim Harris

ETH zürich

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Introduction

Lattice QCD measurements of $(g-2)_\mu$, f_K/f_π, g_A, $\sqrt{t_0}$, ... now achieve $\sim 1\%$ precision

To go beyond this accuracy, QCD with $m_u = m_d$ may not be sufficent

Common approaches to include QED

- simulate QCD+QED in a Monte Carlo
- expand in $\alpha \approx 1/137$ and $(m_u^R - m_d^R)/\Lambda_{QCD} \sim 1\%$

> *...electro-quenched simulations are expected to have an O(10%) accuracy for the leading electromagnetic effects. This suppression is in principle rather weak and results obtained from electro-quenched simulations might feature uncontrolled systematic errors*
>
> *–FLAG2021*

[1] **Borsanyi:2020mff**; **Bushnaq:2022aam**; **CSSM:2019jmq**; **Aoki:2012st**; **PhysRevLett.109.072002**.

Introduction

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To go beyond this accuracy, QCD with $m_\mathrm{u} = m_\mathrm{d}$ may not be sufficent

Common approaches to include QED

- simulate QCD+QED in a Monte Carlo
  💰 requires generation of new gauge configurations
- expand in $\alpha \approx 1/137$ and $(m_\mathrm{u}^\mathrm{R} - m_\mathrm{d}^\mathrm{R})/\Lambda_\mathrm{QCD} \sim 1\%$
  📚 increases number and complexity of measurements

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RM123 method

Expanding the path integral $S = S_{\text{QCD}} + \mathrm{i}e \int J_\mu A_\mu$ in $e = \sqrt{4\pi\alpha}$

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

the leading corrections are correlators

$$\frac{\partial}{\partial e} \frac{\partial}{\partial e} \langle O \rangle = (-\mathrm{i})^2 \int_{x,y} \langle J_\mu(x) A_\mu(x) J_\nu(y) A_\nu(y) O \rangle_{\text{conn}}$$

with two insertions of the electromagnetic current

$$J_\mu = \frac{2}{3} \bar{u} \gamma_\mu u - \frac{1}{3} \bar{d} \gamma_\mu d - \frac{1}{3} \bar{s} \gamma_\mu s,$$

E.g. corrections to the spectrum, we need the insertion with a two-point function

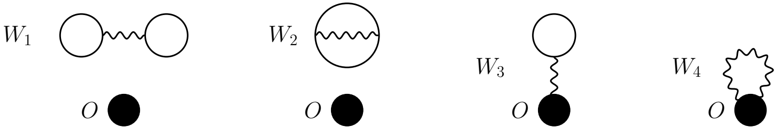
$$O = \int \mathrm{d}^3 x \, \phi_\pi(x) \phi_\pi^\dagger(0)$$

from which we can extract m_{π^+} etc.

[2] **deDivitiis:2011eh**; **deDivitiis:2013xla**.

Leading-order Wick contractions

The fields contract within the currents ($W_{1,2}$), or with fields in the operator O ($W_{3,4}$)



e.g. $W_{1,2}$ are expressed in terms of the photon propagator $G^{\mu\nu}$ (in fixed gauge)

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

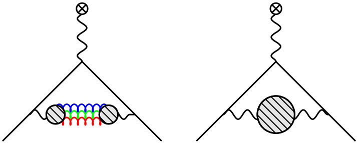
where $H_{1,2}$ are the traces of quark propagators $S^f = D_f^{-1}$

$$H_1^{\mu\nu}(x,y) = \sum_{f,g} Q_f Q_g \, \mathrm{tr}\{\gamma_\mu S^f(x,x)\} \, \mathrm{tr}\{\gamma_\nu S^g(y,y)\},$$
$$H_2^{\mu\nu}(x,y) = -\sum_f Q_f^2 \, \mathrm{tr}\{\gamma_\mu S^f(x,y)\gamma_\nu S^f(y,x)\}$$

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

Relation to the LO HVP

The propagator traces $H_{1,2}$ are similar to the ones which define the LO HVP



e.g. for $g-2$ in the time-momentum representation

$$a_\mu^{\mathrm{LO,HVP}} = \left(\frac{\alpha}{\pi}\right)^2 \int \mathrm{d}^4x\, K(x_0, m_\mu) \langle H_1^{ii}(x,0) + H_2^{ii}(x,0)\rangle$$

Replace photon propagator $G(x) \sim x^{-2}$ (small x) $\longrightarrow$ kernel $K \sim x_0^4$ (small x_0)

😀 Good methods exist for evaluating the disconnected traces H_1

[3] **Bernecker:2011gh**.

Outline

1. Disconnected contribution to HVP
   - Analysis of the variance
   - Numerical experiments
   - Extensions for single flavour and $N_{\mathrm{f}} = 1 + 1 + 1$

2. Disconnected contributions to IB
   - Analysis of the variance
   - Numerical experiments

Analysis of the disconnected contribution to LO HVP

The disconnected diagram H_1 factorizes

$$H_1^{\mu\nu}(x,y) = T^\mu(x) T^\nu(y),$$
$$T^\mu(x) = \sum_f Q_f \,\mathrm{tr}\{\gamma_\mu S^f(x,x)\}$$

and so does its variance which parameterizes the std. error $= \sigma/\sqrt{N_{\mathrm{cfg}}}$

$$\sigma_H^2(x,y) = \langle H_1^2 \rangle - \langle H_1 \rangle^2$$
$$\approx \sigma_T^2 \sigma_T^2 \qquad \text{when} \qquad |x-y| \gg m_\pi^{-1}$$

Consider the contribution of a single light flavour, e.g. $f = \mathrm{u}$ with $Q_\mathrm{u} = 1$

The variance of $T_f(x)$ can be re-expressed in terms of local operators

$$\sigma_{T_f}^2 = \langle V_\mu^{\mathrm{uu}}(0) V_\mu^{\mathrm{dd}}(0) \rangle \sim a^{-6}$$

so is dominated by short-distance fluctuations as $a \to 0$

[4] Giusti:2019kff.

Translation averaging (and its approximations)

Suppose we compute the translation-average over L^3

$$\bar{T}^{\mu}_{f}(x_0) = \frac{a^3}{L^3}\sum_{\vec{x}} T^{\mu}_{f}(x)$$

then its variance is suppressed by the spatial volume

$$\sigma^2_{\bar{T}_f} = \frac{a^3}{L^3}\Big[\sigma^2_{T_f} + \sum_{\vec{x}\neq\vec{0}}\langle V^{\rm uu}_{\mu}(x)V^{\rm dd}_{\mu}(0)\rangle_{\rm conn.}\Big] \sim \frac{a^3}{L^3}a^{-6} \sim a^{-3}$$

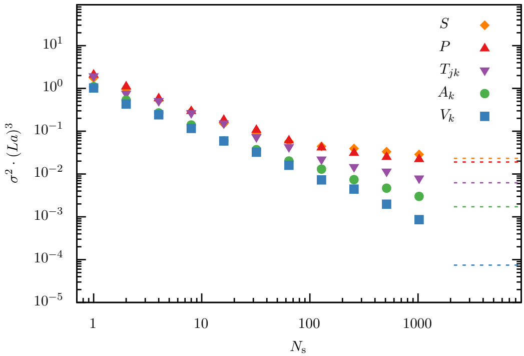
However, we can only compute estimators like the Hutchinson trace

$$\bar{\mathcal{T}}^{\mu}_{f}(x) = \frac{1}{N_{\rm src}}\sum_{i=1}^{N_{\rm src}} \eta_i^{\dagger}(x)\{S_f\eta_i\}(x)$$

which introduce additional variance due to the fluctuations of η

$$\begin{aligned}\sigma^2_{\bar{\mathcal{T}}_f} &= \sigma^2_{\bar{T}_f} + \sigma^2_{\rm s} \\ &= \text{“gauge noise”} + \frac{1}{N_{\rm src}} \times \text{“random field noise”}\end{aligned}$$

Numerical experiment



$N_f = 2$ O(a)-improved Wilson fermions $m_\pi = 270\,\text{MeV}$ $m_\pi L = 4.3$

Using gaussian auxiliary fields, the total variance is

$$\sigma^2_{\mathcal{T}_f} = \frac{a^3}{L^3} \sum_{\vec{x}} \left[\langle V_\mu^{\rm uu}(x) V_\mu^{\rm dd}(0) \rangle + \frac{1}{N_{\rm src}} \langle P^{\rm ud}(x) P^{\rm du}(0) \rangle \right]$$

Including $N_\mathrm{f} = 2+1$ $\mathrm{u,d,s}$ flavours

With $m_\mathrm{u} = m_\mathrm{d}$ and $Q_\mathrm{u} = \frac{2}{3}$, $Q_\mathrm{d} = Q_\mathrm{s} = -\frac{1}{3}$ in the current J_μ

$$\sum_{f=\mathrm{u,d,s}} Q_f S_f = \tfrac{1}{3}\{S_\mathrm{ud} - S_\mathrm{s}\}$$

Using the identity $S_\mathrm{ud} - S_\mathrm{s} = (m_\mathrm{s} - m_\mathrm{ud}) S_\mathrm{ud} S_\mathrm{s}$

1. the variance is suppressed comapared to the single flavour

$$\sigma^2_{\mathcal{T}} \sim (m_\mathrm{ud} - m_\mathrm{s})^2 a^{-1} \qquad \text{as} \qquad a \to 0$$

2. there are two independent estimators for the difference

$$\Theta_\mu(x) = \tfrac{1}{3}(m_\mathrm{s} - m_\mathrm{ud}) \frac{1}{N_\mathrm{src}} \sum_{i=1}^{N_\mathrm{src}} \eta_i^\dagger(x) \gamma_\mu \{S_\mathrm{ud} S_\mathrm{s} \eta_i\}(x),$$

$$\mathcal{T}_\mu(x) = \tfrac{1}{3}(m_\mathrm{s} - m_\mathrm{ud}) \frac{1}{N_\mathrm{src}} \sum_{i=1}^{N_\mathrm{src}} \{\eta_i^\dagger S_\mathrm{s}\}(x) \gamma_\mu \{S_\mathrm{ud} \eta_i\}(x)$$

where the cyclicity of the trace is used in the second “split-even” estimator

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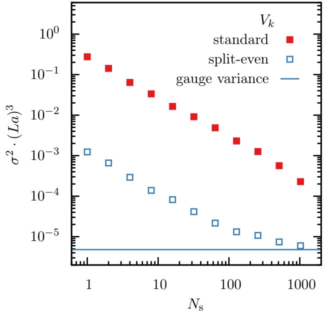
[5] **ETM:2008zte**.

Numerical experiment with $N_\mathrm{f} = 2 + 1$ u, d, s flavours



Observations

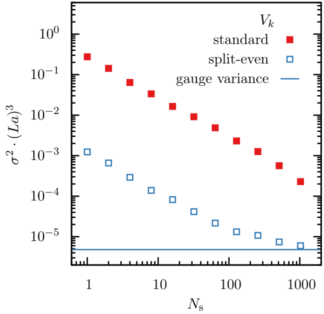
1. the total variance is suppressed w.r.t. single flavour, as expected
2. the gauge noise $\lll$ random field noise as before
3. the split-even estimator has much smaller random field noise

The additional contribution from the auxiliary fields

$$\sigma^2_{\tilde{\Theta}} = \sigma^2_{\bar{T}} - \frac{(m_\mathrm{s} - m_\mathrm{ud})^2}{L^3} \frac{1}{N_\mathrm{src}} a^{11} \sum_{x,y,z} \langle P^\mathrm{ud}(x) S^\mathrm{ds}(y) P^\mathrm{sc}(z) S^\mathrm{cu}(0) \rangle$$

$$\sigma^2_{\tilde{T}} = \sigma^2_{\bar{T}} - \frac{(m_\mathrm{s} - m_\mathrm{ud})^2}{L^3} \frac{1}{N_\mathrm{src}} a^{11} \sum_{x,\vec{y},z} \langle P^\mathrm{ud}(x) V^\mathrm{ds}_\mu(0,\vec{y}) P^\mathrm{sc}(z) V^\mathrm{cu}_\mu(0) \rangle$$

Numerical experiment with $N_\mathrm{f} = 2+1$ u, d, s flavours



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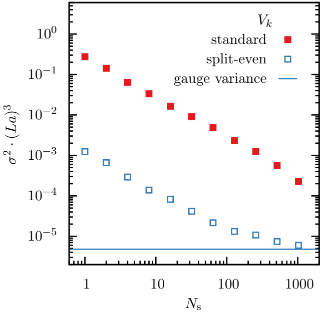

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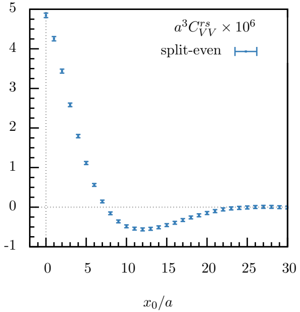
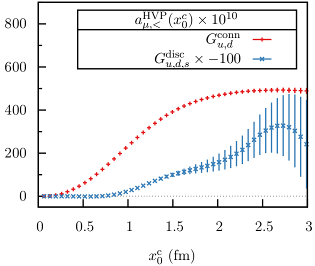
$$\sigma^2_{\mathcal{T}} = \sigma^2_{\bar{T}} - \frac{(m_\mathrm{s} - m_\mathrm{ud})^2}{L^3} \frac{1}{N_\mathrm{src}} a^{11} \sum_{x,\color{blue}{\vec{y}}\color{black},z} \langle P^\mathrm{ud}(x) V^\mathrm{ds}_\mu(0,\vec{y}) P^\mathrm{sc}(z) V^\mathrm{cu}_\mu(0) \rangle$$

$N_\mathrm{f} = 2+1$ contribution to $a_\mu^{\mathrm{LO,HVP}}$

Excellent signal for the disconnected contribution to $a_\mu^{\mathrm{LO,HVP}}$ up to $\sim 2.5\,\mathrm{fm}$

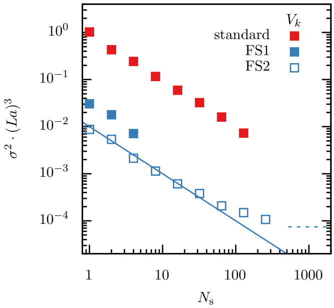




Factor O(100) reduction in the cost compared to the standard estimator

Using $N_{\mathrm{src}} \sim \mathrm{O}(1000)$ average we compute the correlator with full translation averaging

Extensions for single flavour



An improved estimator for a single flavour can be built by splitting, e.g.

$$S_{ud} = (S_{ud} - S_s) + (S_s - S_c) + S_c$$

The hopping parameter expansion is efficient for $m_q \gtrsim m_c$

Using probing vectors the first few terms can also be computed exactly

A factor $O(10 - 20)$ reduction in the cost after accounting for the additional inversions

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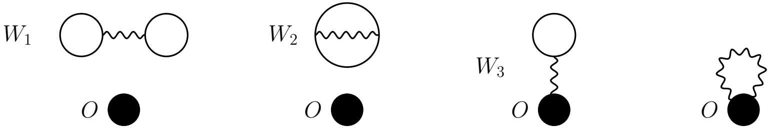
QCD+QED with charged sea quarks



These diagrams are to be evaluated in the $N_\mathrm{f} = 2+1$ theory

⚠️ Physical predictions from QCD+QED require all diagrams including mass insertions

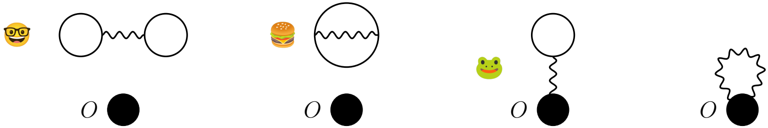
In the following we assume the photon in Feynman gauge and $\mathrm{QED_L}$ prescription

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

⚠️ Ignore pathologies in this formulation due to non-locality.

[6] **Hayakawa:2008an**.

QCD+QED with charged sea quarks



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Analysis of the variance of W_1 contribution

The leading corrections are defined by fully-connected correlators

$$\frac{\partial}{\partial e}\frac{\partial}{\partial e}\langle O\rangle\Big|_{e=0} = \langle OW_1\rangle_{\rm conn} + \dots$$
$$= \langle OW_1\rangle - \langle O\rangle\langle W_1\rangle + \dots$$

Assuming the fields to be gaussian, the variance factorizes

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

where we assume the variance is larger than the signal $\langle OW_1\rangle_{\rm conn}$

For a single flavour, the variance is dominated by the short-distance contribution

$$\sigma^2_{W_1} \sim a^{12}\underbrace{\langle A_\mu A_\nu A_\rho A_\sigma V^{\rm uu}_\mu V^{\rm dd}_\nu V^{\rm u'u'}_\rho V^{\rm d'd'}_\sigma\rangle}_{a^{-16}} \sim a^{-4} \qquad \text{as} \qquad a \to 0$$

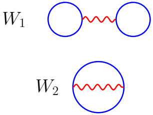
and similarly for W_2

Translation averaging

To implement full translation averaging, we need to introduce stochastic estimators for

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

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



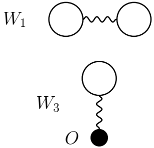
which determine $W_{1,2}$ by the convolution with photon propagator $G^{\mu\nu}$

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

💡 Compute the convolution exactly and avoid stochastic photon fields

$W_{1,3}$ quark-line disconnected

W_1 and W_3 contain the same trace $T(x)$ that appeared in the LO HVP



Including $N_\mathrm{f} = 2 + 1$ flavours the variance

$$\sigma^2_{W_1} \sim (m_\mathrm{s} - m_\mathrm{ud})^4$$

Use the split-even estimator $\mathcal{T}_\mu(x)$

$$\mathcal{W}_1 \approx a^8 \sum_x \mathcal{T}_\mu(x) \Big(\sum_y G_{\mu\nu}(x-y) \mathcal{T}_\nu(y) \Big)$$

where the convolution $a^4 \sum_y G_{\mu\nu}(x-y) T_\nu(y)$ can be computed in Fourier space

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

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

Numerical set-up

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

Table: C1 Ensemble

QCD configurations generated by the RBC/UKQCD configuration

- $N_{\mathrm{f}} = 2 + 1$ domain-wall fermions $\rightsquigarrow$ chiral regularization
- local discretization of the current

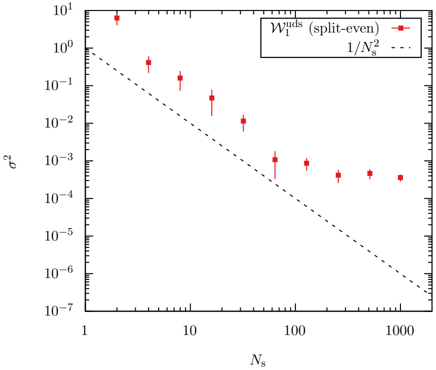
😃 The identity

$$S_{\mathrm{ud}} - S_{\mathrm{s}} = (m_{\mathrm{s}} - m_{\mathrm{ud}}) S_{\mathrm{ud}} S_{\mathrm{s}}$$

holds for the approximation to the overlap operator used here.

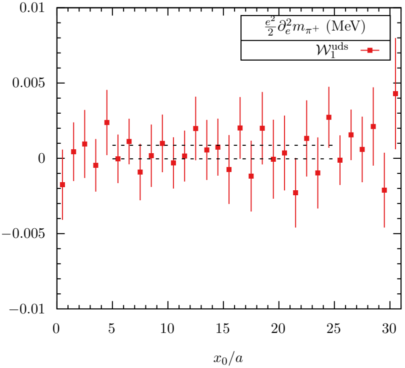
[7] **RBC:2014ntl**.

Numerical experiments W_1 1



- Scaling with $1/N_{\mathrm{src}}^2$
- Saturation of gauge variance with $N_{\mathrm{src}} \sim \mathrm{O}(100)$ inversions

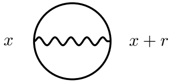
Numerical experiments W_1 2



Correction to charged pion mass due to W_1

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

W_2 quark-line connected



No cancellation of the divergence $\sigma^2_{W_2} \sim a^{-4}$

Need translation averaging for short-distance contribution $r \sim 0$

Compute the all-to-all propagator

$$\mathcal{S}^f(x, x+r) = \frac{1}{N_{\rm src}} \sum_{i=1}^{N_{\rm src}} \{S^f \eta_i\}(x)\eta_i^\dagger(x+r)$$

to create a stochastic estimator

$$\mathcal{H}_2^{\mu\nu}(r) = a^4 \sum_x \sum_f Q_f^2 \mathrm{tr}\{\gamma_\mu \mathcal{S}^f(x, x+r)\gamma_\nu \mathcal{S}^f(x+r, x)\}$$

Introduces a (mild) signal-to-noise ratio problem in r

$\rightsquigarrow$ restrict to $|r| \leq R$

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[8] **deDivitiis:1996qx**.

W_2 quark-line connected

For the remainder $|r| > R$, N_X randomly selected point sources X_n

$$\bar{H}_2^{\mu\nu}(r) = \frac{L^4}{N_X} \sum_{n=1}^{N_X} H_2^{\mu\nu}(X_n, X_n + r)$$

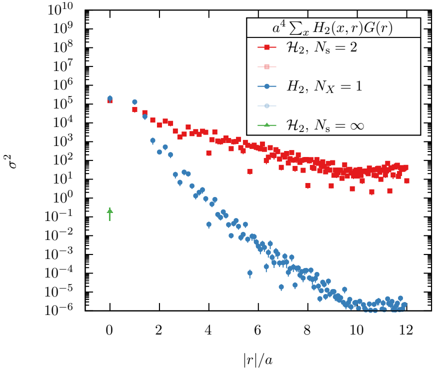
so that the total is split between short- and long-distance

$$\mathcal{W}_2 = a^4 \sum_{|r| \leq R} \mathcal{H}_2^{\mu\nu}(r) G^{\mu\nu}(r) + a^4 \sum_{r > R} \bar{H}_2^{\mu\nu}(r) G^{\mu\nu}(r)$$

Efficient for small r as $\sigma^2_{\mathcal{H}_2} \sim \frac{1}{N^2_{\mathrm{src}}}$

Efficient at large r with no signal-to-noise ratio problem

Numerical experiments W_2 1

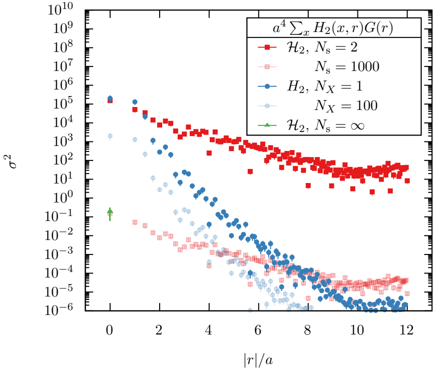


Choose $R/a \sim 4$ so variance is dominated by short-distance contribution

Using naïve scaling, approach gauge noise with

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

Numerical experiments W_2 1



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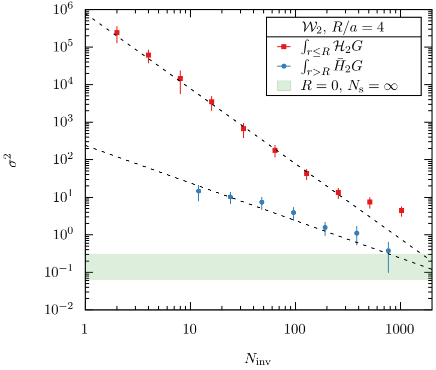
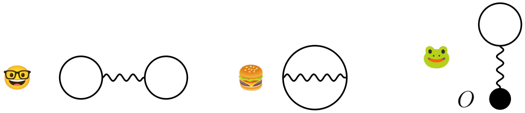


Good scaling of short-distance contribution allows us to approach gauge noise

Long-distance piece under control with moderate cost

Factor $\sim 10^4$ larger variance than W_1

Conclusions



Analysis of the variance helps us construct good estimators

⇝ can substantially reduce cost of translation averaging

For sea-quark electric charge contributions

- $W_{1,3}$ good precision of uds contribution + *split-even* estimator
- W_2 variance dominated by short distances $\sigma^2_{W_2} \sim a^{-4}$

  ⇝ split into short- and long-distance contributions

$W_{1,3}$ are independent of the observable! Worth investing

Next include mass insertions, include corrections close to physical point...