Sea-Quark Isospin-Breaking Effects

Alessandro Cotellucci

Humboldt Universität zu Berlin & DESY Zeuthen, January 22nd 2024

Isospin

Based on the assumption $m_u = m_d$ Isospin is an internal global symmetry which acts as:

$$\begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} \to M \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix} \quad M \in \mathrm{SU}(2).$$

Good approximation as long as the target precision is above 1% in fact:

$$\left(\frac{m_d - m_u}{\Lambda_{\mathrm{QCD}}} \right) \sim 0.01$$

$$e^2 \sim 0.01.$$

Isospin breaking effects

An important phenomenological isospin-breaking effect is the mass difference for Baryons.

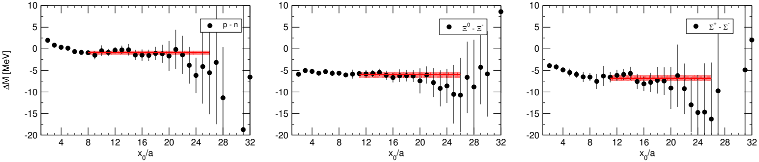


Figure: Effective Baryon mass differences on a $N_f = 1 + 2 + 1$ QCD+QED ensemble[a].

Some observables need isospin-breaking effects to push the precision like $(g-2)_\mu$[b].

[a] Bushnaq et al., "First results on QCD+QED with C* boundary conditions".

[b] Aoyama et al., "The anomalous magnetic moment of the muon in the Standard Model".

QED in Finite Volume

Due to Gauss law:

$$Q_{\text{tot}} = \int_{\text{p.b.c.}} d\vec{x}\ \nabla \cdot \vec{E}\,(\vec{x}) = 0.$$

Possible solutions:

- QED_{L}[c] remove spatial zeroth mode removed from the action,
- QED_{M}[d] massive photon,
- QED_{∞}[e] reconstruction of infinite volume QED,
- QED_{C}[f] modify the boundary conditions.

[c] Hayakawa and Uno, "QED in finite volume and finite size scaling effect on electromagnetic properties of hadrons".

[d] Endres et al., "Massive photons: an infrared regularization scheme for lattice QCD+QED".

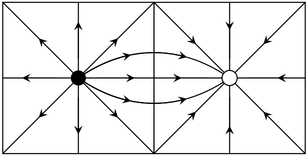
[e] Blum et al., "Using infinite volume, continuum QED and lattice QCD for the hadronic light-by-light contribution to the muon anomalous magnetic moment".

[f] Kronfeld and Wiese, "SU(N) gauge theories with C periodic boundary conditions. 1. Topological structure", "SU(N) gauge theories with C periodic boundary conditions. 2. Small volume dynamics".

C-periodic boundary conditions

Change the spatial boundary conditions to remove the photon zeroth mode.

$$\chi(x) = \begin{pmatrix} \psi(x) \\ \psi^{\mathcal{C}}(x) \end{pmatrix}, \quad \chi(x + L\hat{k}) = K\chi(x).$$



The action in this case is:

$$S = -\frac{1}{2}\sum_x \chi^T KCD\chi, \quad C = i\gamma_0\gamma_2, \quad K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The RM123 method

Reweighting

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

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

[g] Divitiis et al., "Leading isospin breaking effects on the lattice".

The RM123 method

Perturbative expansion

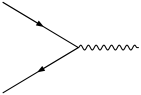
The isospin-breaking action of $N_f = 2$ can be written as:

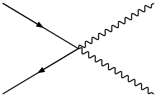
$$
\begin{aligned}
S_{\mathrm{IB}}[U, A, \chi_f] = &- \frac{1}{2} \sum_x \delta m_{ud} \left[\chi_u^T(x) C K \chi_u(x) - \chi_d^T(x) C K \chi_d(x) \right] \\
&- \frac{1}{2} \sum_x \delta m \left[\chi_u^T(x) C K \chi_u(x) + \chi_d^T(x) C K \chi_d(x) \right] \\
&- \frac{1}{8} \sum_{x,\mu\nu,f} \delta c_{\mathrm{SW}}^{\mathrm{SU}(3)f} \chi_f^T(x) C K \sigma_{\mu\nu} \hat{G}_{\mu\nu}(x) \chi_f(x) \\
&+ \delta\beta S_{\mathrm{gluon}}[U] + S_{\mathrm{QED}}[A, U, \chi_f]
\end{aligned}
$$

The RM123 method

Lattice QED Action for $O(a)$ Wilson fermions

$$
\begin{aligned}
S_{\mathrm{QED}}[U, A, \chi_f] =& \frac{e}{8} \sum_{xy,\mu\nu,f} q_f c_{\mathrm{f}} \chi_f^T(x) C K \sigma_{\mu\nu} \widehat{A}_{\mu\nu}(x) \chi_f(x) \\
& - \frac{ie}{2} \sum_{x,f} q_f \chi_f^T(x) J(x,y) \chi_f(y) \\
& + \frac{e^2}{4} \sum_{xy,f} q_f^2 \chi_f^T(x) T(x,y) \chi_f(y)
\end{aligned}
$$





The RM123 method

Photon field

The photon fields are generated starting from the photon path integral:

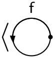
$$\int dA \; e^{-S_\gamma[A]} = \int dA \; e^{-\frac{1}{2}\sum_{k,\mu\nu} \tilde{A}_\mu(k) K_{\mu\nu} \tilde{A}_\nu(k)}$$

$K_{\mu\nu}$ Requires gauge fixing $\rightarrow$ Coulomb Gauge (Necessary for the tuning).
$\tilde{A}_\mu(k)$ Gaussian decorrelated variables.

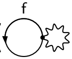
The RM123 method

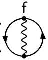
Sea-Sea terms

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

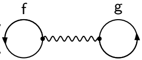
$\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle_{\mathrm{Iso}} - \delta\beta \langle S_{gauge}\mathcal{O} \rangle_{\mathrm{Iso},c} + \sum_f \delta m_f \langle$ 

$\mathcal{O} \rangle_{\mathrm{Iso},c}$

$+ e^2 \Bigg[\sum_f \hat{q}_f^2 \Bigg(\langle$ 

$\mathcal{O} \rangle_{\mathrm{Iso},c} + \langle$ 

$\mathcal{O} \rangle_{\mathrm{Iso},c} \Bigg)$

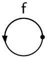
$+ \sum_{fg} \hat{q}_f \hat{q}_g \langle$ 

$\mathcal{O} \rangle_{\mathrm{Iso},c} \Bigg] .$

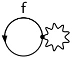
The RM123 method

Sea-Sea Diagrams

$$I^{f}_{mass} = \frac{1}{2}\sum_{x} \text{Re tr}\left[D_f^{-1}(x,x)\right] =$$



$$I^{f}_{tad} = -\frac{1}{4}\sum_{xy} \langle \text{Re tr}\left[D_f^{-1}(x,y)T(y,x)\right]\rangle_\gamma =$$

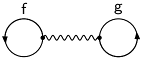


$$I^{fg}_{cur,bub} = \frac{1}{8}\sum_{xyzw,\mu} \langle \text{Im tr}\left[J(x,y)D_f^{-1}(y,x)\right] \text{Im tr}\left[J(z,w)D_g^{-1}(w,z)\right]\rangle_\gamma$$

$$I^{fg}_{sw,bub} = \frac{c_f c_s}{128}\sum_{xy,\mu\nu\rho\sigma} \langle \text{Re tr}\left[\sigma_{\mu\nu}\hat{A}_{\mu\nu}(x)D_f^{-1}(x,x)\right] \text{Re tr}\left[\sigma_{\rho\sigma}\hat{A}_{\rho\sigma}(y)D_g^{-1}(y,y)\right]\rangle_\gamma$$

$$I^{fg}_{mix,bub} = \frac{c_f}{16}\sum_{xyz,\mu\nu} \langle \text{Re tr}\left[\sigma_{\mu\nu}\hat{A}_{\mu\nu}(x)D_f^{-1}(x,x)\right] \text{Im tr}\left[J(y,z)D_g^{-1}(z,y)\right]\rangle_\gamma$$

$=$

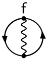


$$I^{f}_{cur,self} = \frac{1}{4}\sum_{xyzw,\mu} \langle \text{Re tr}\left[J(x,y)D_f^{-1}(y,z)J(z,w)D_f^{-1}(w,x)\right]\rangle_\gamma$$

$$I^{f}_{sw,self} = -\frac{c_f^2}{64}\sum_{xy,\mu\nu\rho\sigma} \langle \text{Re tr}\left[\sigma_{\mu\nu}\hat{A}_{\mu\nu}(x)D_f^{-1}(x,y)\sigma_{\rho\sigma}\hat{A}_{\rho\sigma}(y)D_f^{-1}(y,x)\right]\rangle_\gamma$$

$$I^{f}_{mix,self} = -\frac{c_f}{8}\sum_{xyz,\mu\nu} \langle \text{Im tr}\left[\sigma_{\mu\nu}\hat{A}_{\mu\nu}(x)D_f^{-1}(x,y)J(y,z)D_f^{-1}(z,x)\right]\rangle_\gamma$$

$=$



Algorithms

Girard-Hutchinson trace estimator[h]

The trace can be approximated with stochastic sources.

$$\sum_x \mathrm{tr}\left[D^{-1}(x,x)\right] = \mathrm{Tr}\left[D^{-1}\right] = \mathrm{Tr}\left[D^{-1}\mathbb{1}\right]$$

$$= \lim_{N_s \to \infty} \frac{1}{N_s} \sum_i^{N_s} \eta_i^\dagger D^{-1} \eta_i$$

with:

$$\langle \eta \eta^\dagger \rangle = \mathbb{1} \ \& \ \langle \eta \rangle = 0$$

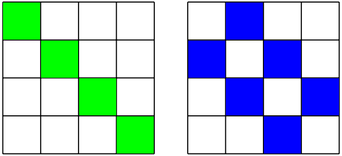
[h] Girard, "A fast 'Monte-Carlo cross-validation' procedure for large least squares problems with noisy data"; Hutchinson, "A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines".

Algorithms

Hopping Expansion

The Wilson-Dirac operator can be rewritten as[i]:

$$D = \underbrace{M} + \underbrace{H} .$$



This method allows one to write:

$$D^{-1} = \left(1 - D^{-1} H\right) M^{-1}$$

This leads to the general order formula:

$$D^{-1} = M^{-1} \sum_{n=0}^{m} \left(-H \ M^{-1}\right)^{n} + D^{-1} \left(-H \ M^{-1}\right)^{m+1}$$

[i] Thron et al., "Padé-Z_2 estimator of determinants".

Algorithms

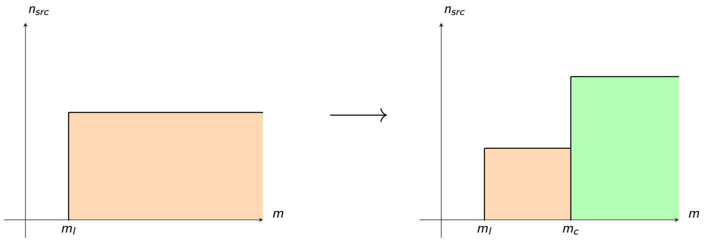
Frequency Splitting

Using the relation:

$$D_{m_i}^{-1} - D_{m_j}^{-1} = (m_j - m_i)\, D_{m_i}^{-1} D_{m_j}^{-1}$$

So one can rewrite[j]

$$D_m^{-1} = \sum_{i=0}^{N-1} (m_{i+1} - m_i) D_{m_i}^{-1} D_{m_{i+1}}^{-1} + D_{m_N}^{-1}$$



[j] Giusti et al., "Frequency-splitting estimators of single-propagator traces".

Ensembles

lattice	a [fm]	m_π [MeV]	m_D [MeV]	no. cnfg	*nsrc* per lv per cnfg
64×32^3	0.05393(24)	398.5(4.7)	1912.7(5.7)	50	400
80×48^3	0.05400(14)	401.9(1.4)	1908.5(4.5)	50	100

Table: Configurations used.

Parameters used:

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

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

$$e = e_{\mathrm{phys}}$$

δm_f from QCD+QED simulation.

From QCD $\mathrm{N}_f = 3 + 1$ to QCD+QED $\mathrm{N}_f = 1 + 2 + 1$.

Scale-Setting

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

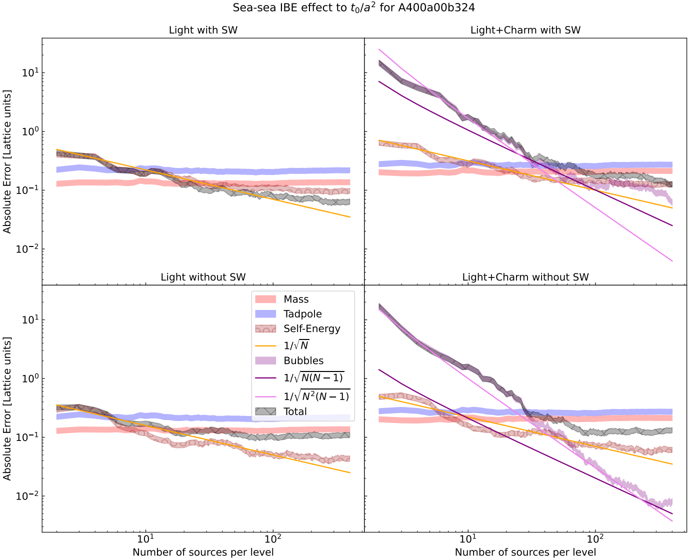
$$t_0^2 \langle E(t) \rangle \Big|_{t=t_0} = 0.3$$

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

Table: IBE effects on t_0 for A400a00b324 (preliminary).

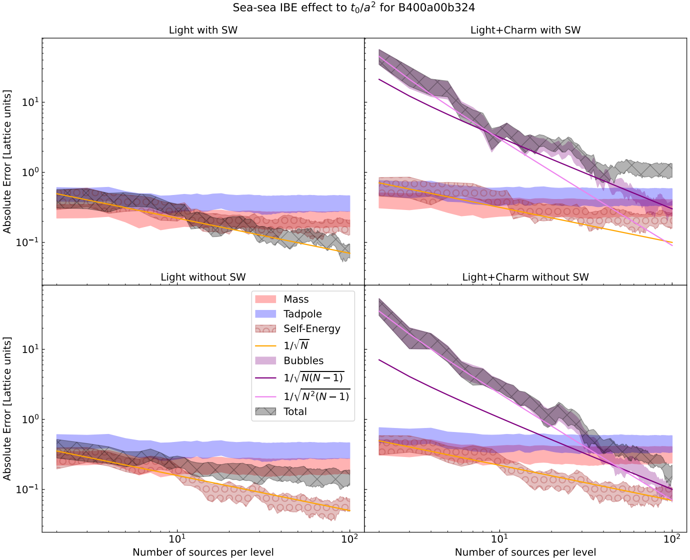
t_0 error on A400a00b324

Function of the number of sources



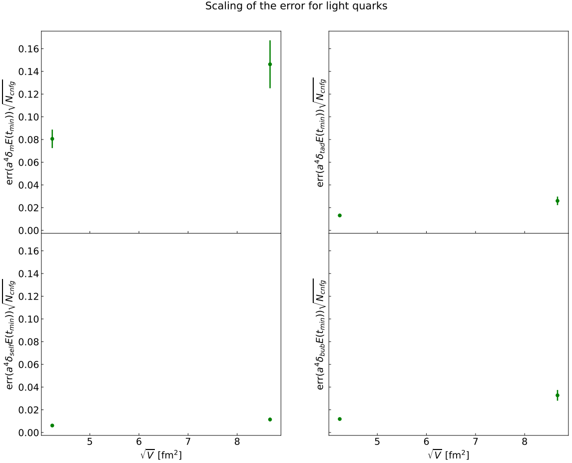
t_0 error on B400a00b324

Function of the number of sources

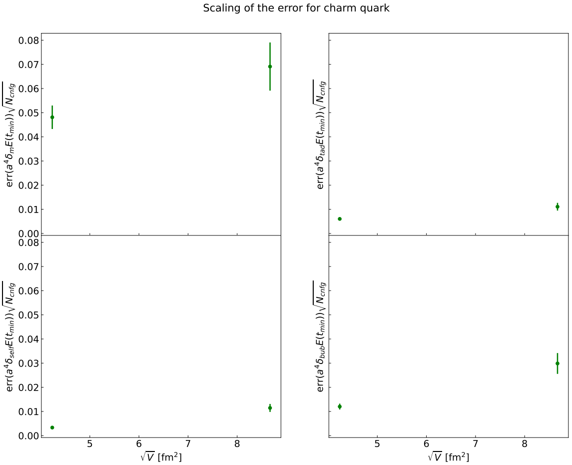


Volume Scaling of the Variance

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.



Volume Scaling of the Variance



Pion mass

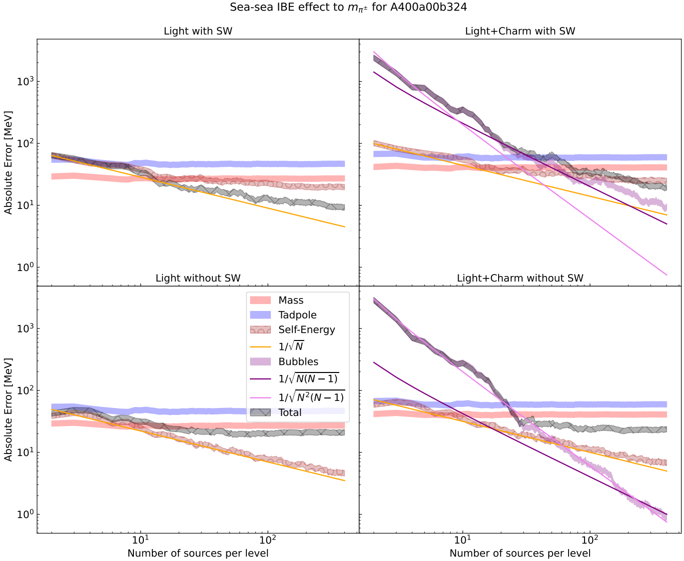
Sea-sea contribution to the pion mass.

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

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

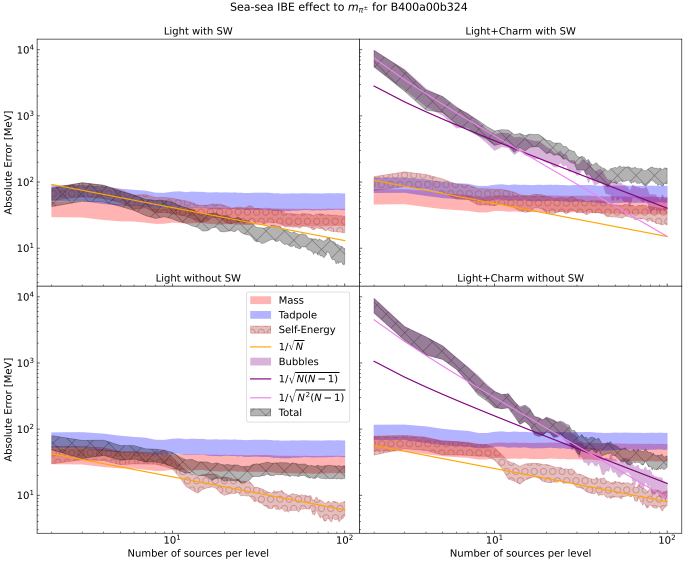
$m_{\pi^\pm}$ error on A400a00b324

Function of the number of sources



$m_{\pi^\pm}$ error on B400a00b324

Function of the number of sources



Conclusion and Outlook

Conclusions:

- ✓ 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;

To do:

- To include the valence-valence and sea-valence to analyse the meson masses;
- To study the scale of the error in $a \to 0$, $V \to \infty$ and $m_\pi \to m_{\pi^{\text{phys.}}}$;
- To evaluate the sea-sea contributions isolating the short and long distance;

Thank you for your attention!

Acknowledgments

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

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Backup

Mass Term Estimator

The mass term has been estimated using the following method:

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

Backup

Tadpole Term Estimator

The tadpole term has been estimated using the following method:

$$
\begin{aligned}
\mathrm{Tr}\left[TD_{m_u}^{-1}\right] \sim (m_c - m_u)\,\frac{1}{N_s}\sum_{i}^{N_s}\left(D_{m_c}^{\dagger}\eta_i\right)^{\dagger} TD_{m_u}\eta_i \\
+ \sum_{i}^{N_{pr}} s_i^{\dagger}\, TSW^{-1}\sum_{n=0}^{2}\left(-HSW^{-1}\right)^{n} s_i \\
+ \frac{1}{N_s}\sum_{i}^{N_s}\xi_i^{\dagger}\, T\left(-SW^{-1}H\right)^{3} D_{m_c}^{-1}\xi_i
\end{aligned}
$$

Backup

Bubbles Estimator

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

$$\left[JD_{m_c}^{-1}\right]_i^a = \sum_j^{N_{pr}} s_j^\dagger J^a SW^{-1} \sum_{n=0}^{2} \left(-HSW^{-1}\right)^n s_j + \xi_i^\dagger J^a \left(-SW^{-1}H\right)^3 D_{m_c}^{-1} \xi_i$$

$$\left[\sigma_{\mu\nu}\hat{A}_{\mu\nu} D_{m_c}^{-1}\right]_i^a = \sum_j^{N_{pr}} s_j^\dagger \sigma_{\mu\nu}\hat{A}_{\mu\nu}^a SW^{-1} \sum_{n=0}^{3} \left(-HSW^{-1}\right)^n s_j + \xi_i^\dagger \sigma_{\mu\nu}\hat{A}_{\mu\nu}^a \left(-SW^{-1}H\right)^4 D_{m_c}^{-1} \xi_i$$

The stochastic estimator will be:

$$\mathrm{Tr}\left[JD_{m_c}^{-1}\right] \mathrm{Tr}\left[JD_{m_c}^{-1}\right] \sim \frac{2}{N_s\left(N_s-1\right)} \sum_{i\neq j}^{N_s} \frac{1}{N_A} \sum_a^{N_A} \left[JD_{m_c}^{-1}\right]_i^a \left[JD_{m_c}^{-1}\right]_j^a$$

Backup

Self-Energy Estimator

The tadpole term has been estimated using the following method:

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

Backup

Gauge Choice

Considering the Gauge-invariant interpolating operator:

$$\Psi^c(x) = \exp\left\{-i\int d^3y\Phi\left(\vec{x}-\vec{y}\right)\partial_k A_k\left(x_0,\vec{y}\right)\right\}\psi(x)$$

with $\partial_k\partial_k\Phi\left(\vec{x}\right) = \delta^3\left(\vec{x}\right)$ In Coulomb gauge, it is just $\psi(x)$.
Considering the Gauge-invariant interpolating operator:

$$\Psi^l(x) = \exp\left\{-i\int d^4y\Phi\left(x-y\right)\partial_\mu A_\mu\left(y\right)\right\}\psi(x)$$

with $\partial_\mu\partial_\mu\Phi\left(x\right) = \delta^4\left(x\right)$ In Landau gauge it is just $\psi(x)$.
If one is interested in extracting the mass from the gauge fixed operator:

$$\sum_{\vec{x}}\langle\psi(t,\vec{x})\bar{\psi}(0)\rangle = \sum_{\vec{x}}\langle\psi(0,\vec{x})e^{-tH}\bar{\psi}(0)\rangle \sim Ae^{-tm_\psi}$$

Backup

Gauge Choice

In Landau gauge, this is equivalent to extracting the mass from:

$$\sum_{\vec{x}} \langle \Psi^{l}(t, \vec{x}) \bar{\Psi}^{l}(0) \rangle$$

In Coulomb gauge from:

$$\sum_{\vec{x}} \langle \Psi^{c}(t, \vec{x}) \bar{\Psi}^{c}(0) \rangle$$