QCD + QED studies using Twist-Averaging

Christoph Lehner (BNL)

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QCD + QED studies using Twist-Averaging

Taku Izubuchi and Christoph Lehner (PI)

Project homepage:
`http://quark.phy.bnl.gov/~clehner/usqcd/ta/`

Collaborators: Tom Blum, Norman Christ, Tomomi Ishikawa, Luchang Jin, and Amarjit Soni

(RBC collaboration)

Abstract

We propose a dedicated effort to study QED corrections and in particular finite-volume artifacts for the QED pion mass splitting Δm_π, f_π, and the hadronic light-by-light contribution to $(g-2)_\mu$. We will explore a new method recently suggested by some of the authors that promises to reduce finite-volume errors in these computations. **We request 27.3 Mio Jpsi-equivalent core-hours on the Fermilab clusters and 17 (806) TB of disk (tape) space at Fermilab. The total cost of this project therefore is 30.1 Mio Jpsi-equivalent core-hours.**

LATTICE QCD AT THE INTENSITY FRONTIER

Thomas Blum, Michael Buchoff, Norman Christ, Andreas Kronfeld,
Paul Mackenzie, Stephen Sharpe, Robert Sugar and Ruth Van de Water

(USQCD Collaboration)

(Dated: October 22, 2013)

IV. FUTURE LATTICE CALCULATIONS

A second advance will be the systematic inclusion of isospin-breaking and electromagnetic (EM) effects. Once calculations attain percent-level accuracy, as is the case at present for quark masses, f_K/f_π, the $K \to \pi$ and $B \to D^*$ form factors, and $\hat{B}_K$, one must study the effects of EM and isospin breaking. A partial and approximate inclusion of such effects is already made for light quark masses, f_π, f_K and $\hat{B}_K$. Full inclusion would require nondegenerate u and d quarks and the incorporation of QED into the simulations. For some quantities it may suffice to implement this only for the valence quarks (quenched QED), while in general one must also include mass differences and electrical charges for the sea quarks. One approach for both isospin and unquenched QCD+QED simulations is to reweight pure QCD

configurations [44, 45]. One concern with QED is that the finite-volume effects will be enhanced due to the masslessness of the photon. In practice, to date, these effects seem to be controllable.

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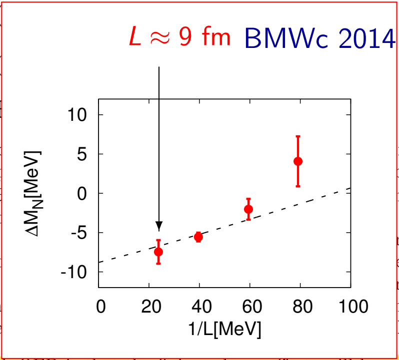

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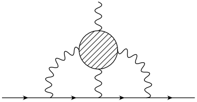
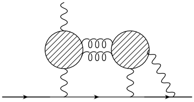
1. Muon anomalous magnetic moment[2]

The muon anomalous magnetic moment provides one of the most precise tests of the Standard Model of particle physics (SM) and often places important constraints on new theories beyond the SM [1]. The current discrepancy between experiment and the Standard Model has been reported in the range of 2.9–3.6 standard deviations [77–79]. With new experiments planned at Fermilab (E989) and J-PARC (E34) that aim to improve on the current 0.54 ppm measurement at BNL [80] by at least a factor of 4, it will continue to play a central role in particle physics for the foreseeable future.





Contribution	Central Value $\times 10^{10}$	Uncertainty $\times 10^{10}$
a_μ^{QED}	11 658 471.895	0.008
a_μ^{EW}	15.4	0.1
$a_\mu^{\mathrm{HAD,\ LO\ VP}}$	* 692.3	4.2
$a_\mu^{\mathrm{HAD,\ HO\ VP}}$	-9.84	0.06
$a_\mu^{\mathrm{HAD,\ LBL}}$	** 10.5	2.6
a_μ^{SM}	11 659 180.3	4.9
FNAL E989 target		≈ 1.6

Introduction to the method

QCD setup

arXiv:1503.04395

$U_\mu(x)$ $\Psi(x+\hat{L}_1+\hat{L}_2)$	$U_\mu(x)$ $\Psi(x+2\hat{L}_1+\hat{L}_2)$	$U_\mu(x)$ $\Psi(x+3\hat{L}_1+\hat{L}_2)$
$U_\mu(x)$ $\Psi(x+\hat{L}_1)$	$U_\mu(x)$ $\Psi(x+2\hat{L}_1)$	$U_\mu(x)$ $\Psi(x+3\hat{L}_1)$

Valence fermions Ψ living on a repeated gluon background U_μ with periodicity L_1, L_2 and vectors $\hat{L}_1 = (L_1, 0)$, $\hat{L}_2 = (0, L_2)$

Let ψ^θ be the quark fields of your finite-volume action with twisted-boundary conditions

$$\psi^\theta_{x+L} = e^{i\theta}\psi^\theta_x \,.$$

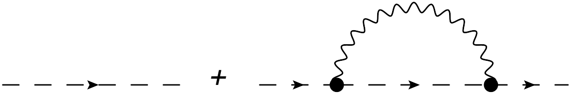
Then one can show that

$$\left\langle \Psi_{x+nL}\bar{\Psi}_{y+mL}\right\rangle = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{i\theta(n-m)} \left\langle \psi^\theta_x \bar{\psi}^\theta_y \right\rangle \,, \qquad (1)$$

where the $\langle\cdot\rangle$ denotes the fermionic contraction in a fixed background gauge field $U_\mu(x)$. (4d proof available.)

This specific prescription produces exactly the setup of the previous page, it allows for the definition of a conserved current, and allows for a prescription for flavor-diagonal states.

Example: QED mass correction on a lattice in finite volume



$$C(p) \quad = \quad \frac{1}{\overline{p}^2 + m^2} \; + \; \alpha \sum_{k \in \mathrm{BZ}^4} \frac{1}{\overline{p}^2 + m^2} \frac{1}{\overline{(p-k)}^2 + m^2} \frac{1}{\overline{p}^2 + m^2} \frac{1}{\overline{k}^2}$$

with $\overline{p}_\mu = 2\sin(p_\mu/2)$

Strategy: compute $C(x) = \sum_{p \in \mathrm{BZ}^4} e^{ipx} C(p)$ in finite-volume and perform effective-mass fit

Twist-averaged version:

$$e^{ik(y+mL)}\left\langle \Psi_{x+nL}\bar{\Psi}_{y+mL}\right\rangle \left\langle \Psi_{y+mL}\bar{\Psi}_{z+lL}\right\rangle$$
$$= \int_0^{2\pi}\frac{d\theta}{2\pi}\int_0^{2\pi}\frac{d\theta'}{2\pi}e^{ik(y+mL)}e^{i\theta(n-m)+i\theta'(m-l)}\left\langle \psi_x^\theta\bar{\psi}_y^\theta\right\rangle \left\langle \psi_y^{\theta'}\bar{\psi}_z^{\theta'}\right\rangle ,$$

Perform sum over m using Poisson's summation formula yields

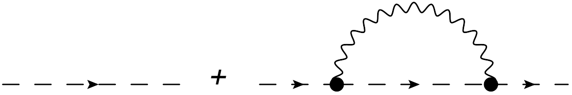
$$\sum_m e^{ik(y+mL)}\left\langle \Psi_{x+nL}\bar{\Psi}_{y+mL}\right\rangle \left\langle \Psi_{y+mL}\bar{\Psi}_{z+lL}\right\rangle$$
$$= e^{iky}\int_0^{2\pi}\frac{d\theta}{2\pi}\int_0^{2\pi}\frac{d\theta'}{2\pi}e^{i\theta n-i\theta' l}\hat{\delta}(k-(\theta-\theta')/L)\left\langle \psi_x^\theta\bar{\psi}_y^\theta\right\rangle \left\langle \psi_y^{\theta'}\bar{\psi}_z^{\theta'}\right\rangle ,$$

with $\hat{\delta}(k) = \frac{2\pi}{L}\sum_{n\in\mathbb{N}}\delta(k+2\pi n/L)$.

TA yields momentum conservation of twists

Example: QED mass correction on a lattice in finite volume

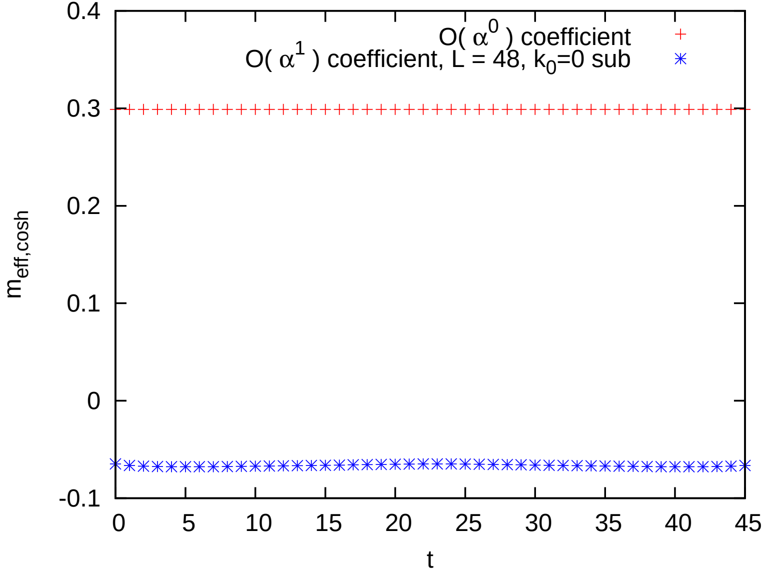
plus TA



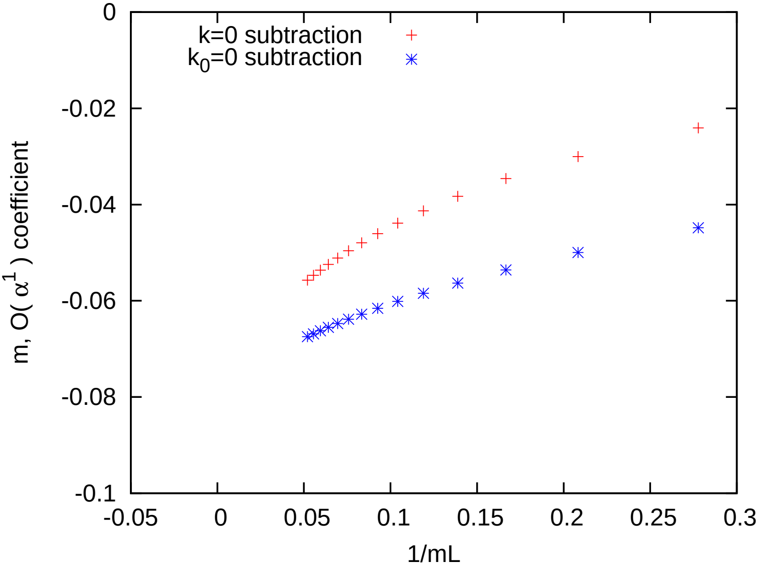
$$C(p) \quad = \quad \frac{1}{\overline{p}^2 + m^2} + \alpha \left\langle \sum_{k \in \mathrm{BZ}^4} \frac{1}{\overline{p}^2 + m^2} \frac{1}{(\overline{p - k'})^2 + m^2} \frac{1}{\overline{p}^2 + m^2} \frac{1}{\overline{k'}^2} \right\rangle_{\theta^4}$$

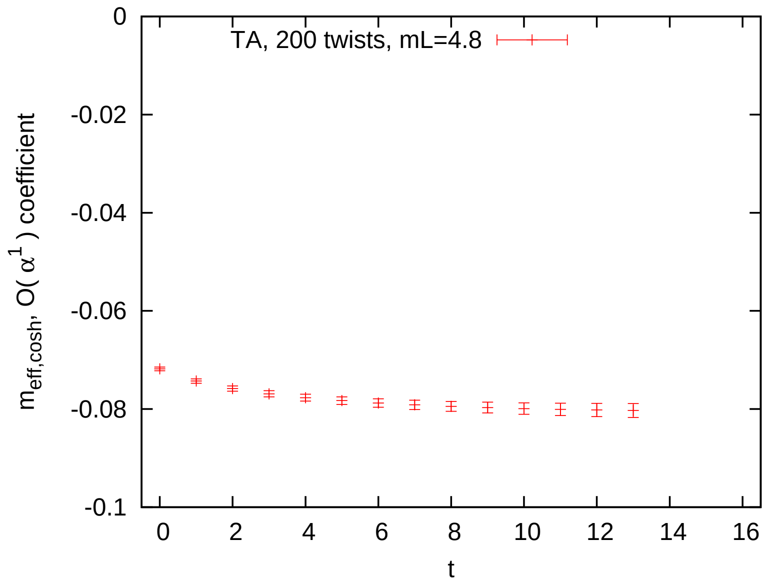
with $\overline{p}_\mu = 2\sin(p_\mu/2)$ and $k'_\mu = k_\mu + \theta_\mu/L_\mu$

Strategy: compute $C(x) = \sum_{p \in \mathrm{BZ}^4} e^{ipx} C(p)$ in finite-volume and perform effective-mass fit

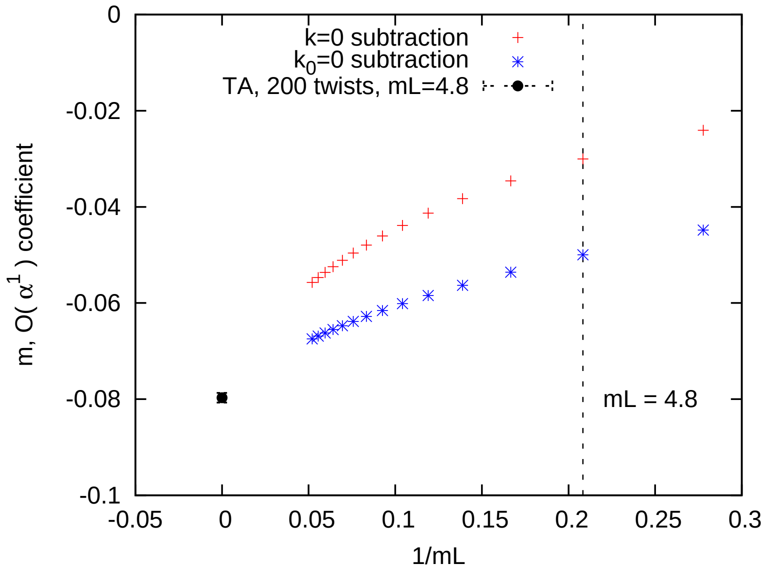


O(α^0) coefficient
O(α^1) coefficient, L = 48, k_0=0 sub
0.4
0.3
0.2
0.1
0
-0.1
0
5
10
15
20
25
30
35
40
45
t
m_eff,cosh


k=0 subtraction
k0=0 subtraction
m, O(α1) coefficient
1/mL
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.05
0
0.05
0.1
0.15
0.2
0.25
0.3



TA, 200 twists, mL=4.8
0
-0.02
-0.04
-0.06
-0.08
-0.1
0
2
4
6
8
10
12
14
16
t
$m_{eff,cosh}$, O(α^1) coefficient



k=0 subtraction
k_0=0 subtraction
TA, 200 twists, mL=4.8
mL = 4.8
m, O(α^1) coefficient
1/mL
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.05
0
0.05
0.1
0.15
0.2
0.25
0.3

Proposed studies

Proposed studies

$\boldsymbol{\Delta m_\pi}$

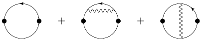


Figure 4: Quark-connected electro-magnetic mass splitting diagrams.

$\boldsymbol{f_\pi}$

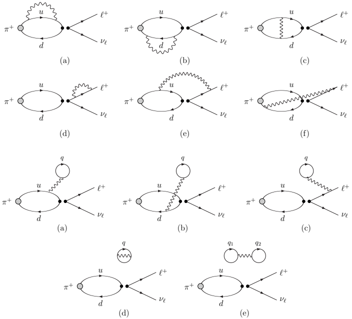


Figure 5: Quark-connected (top) and quark-disconnected (bottom) diagrams for f_π.

$\boldsymbol{(g-2)_\mu}$ HLbL

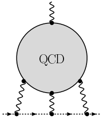


Figure 7: Light-by-light contribution to $(g-2)_\mu$

Carrasco et al. 2015

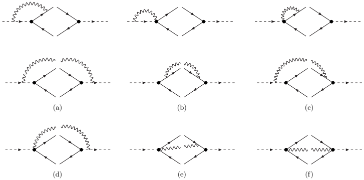


Figure 6: Soft-photon emission in effective field theory.

Main focus of this proposal

1. Volume-dependence of QCD + QED simulations using the TA method

2. Control stochastic noise introduced by twisting

For 1) we propose a study on RBC's 16c and 24c ensemble for $a^{-1} = 1.73$ GeV and $m_\pi = 422$ MeV (all parameters identical apart from volume).

For 2) we propose the computation on the new RBC ensemble 17 (32c, DSDR, zMobius, $a^{-1} = 1.15$ GeV, $m_\pi = 140$ MeV)

In the future we hope to complete this study by generating a partner ensemble for the 32c ensemble to study the volume-dependence at physical pion mass.

Strategy

Two methods are explicitly spelled out in the proposal:

- P+A twist averaging in spatial directions which will be safe regarding 2) but may not achieve the goals in 1)
- Full stochastic twist averaging which has a higher probability to achieve the goals in 1) but may suffer from 2)

The proposal main text explicitly works out a strategy using stochastic A2A propagators

SPC questions

1. *Table 1 only appears to include the cost estimate for a single ensemble (the* 32^3 *DSDR with mpi 135 MeV and 1/a=1.1 GeV). What is the estimated cost for analyzing the other ensembles? Given that you plan to test multiple methods on the* 16^3 *ensemble, presumably this cost, although small, is not negligible.*

```
The cost for the $m_pi=420 MeV$, 24c ensemble is

  Lanczos           1.2 hours    on   1024 BC1 cores    (compared to 28.7 hours for the 32c)
  Exact solve       0.07 hours   on   1024 BC1 cores    (compared to 1.13 hours for the 32c)
  Sloppy solve      0.02 hours   on   1024 BC1 cores    (compared to 0.21 hours for the 32c)

The cost for the 16c ensemble is estimated to be 16^3*32/(24^3*64) \approx 0.15 the cost of
the 24c ensemble.

Therefore even performing two complete runs (say for full stochastic versus PBC+APBC) on the
16c will only add 0.4 Mio Jpsi-core hours to the total budget.  Even very conservatively
estimating the cost of extensive experimentation on the 16c ensemble to be 1 Mio Jpsi-core hours,
combined with the final-volume study of the best method on the 24c ensemble, will yield a total
cost of the 16c and 24c studies that is only 8% of the total requested allocation.
```

2. *Your initial study at two spatial volumes with fixed parameters will use an unphysically heavy pion of mpi $\approx$ 422 MeV. How does the use of such a very heavy pion mass impact the interpretation of the results of your study? In particular, will it potentially change the outcome of which approach (e.g. stochastic versus PBC+APBC) appears more promising?*

See, e.g., slide 2: dashed line is analytic function only of mL. For the study of the volume-dependence we expect to obtain reliable answers from the 16c/24c studies. For the noise study, the 32c ensemble is essential.

3. *It will be very difficult to draw strong conclusions about finite-volume effects with only two spatial volumes at fixed other parameters. Why aren't you planning on analyzing a third ensemble with a different spatial volume and fixed other parameters? (For example, you could analyze a smaller-volume ensemble where the effects are extremely easy to observe, and which would be relatively inexpensive.)*

See slide 11: We hope that mapping out functional dependence is not necessary since we may only see a reasonably small difference between 16c and 24c studies after using TA. If necessary, we will consider generating a third volume such as suggsted by the SPC.

4. *The aim of this proposal is to understand finite-volume errors in lattice QED simulations, and to test methods for reducing these FV errors. How does analyzing the* 32^3 *physical-mass ensemble, which is not at the same parameters as the* 16^3 *and* 24^3 *ensembles help you to achieve this goal?*

See slide 13: For the FV-dependence study the 16c vs 24c test may be an economical way to get a reliable answer. For the noise study the 32c is essential. The long-term goal is to add another partner ensemble to the 32c ensemble to study volume-dependence at physical pion mass.

Thank you

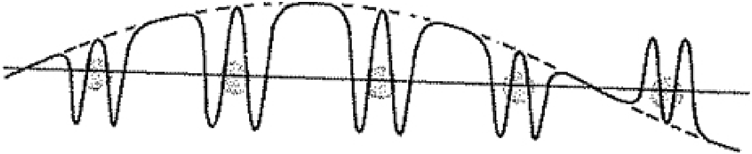
We summarize the cost in Tab. 1. We intend to run using the Clusters at FNAL.

Lanczos for 2000 EV on ensemble 17 on 1024 BC1 cores	28.7 hours
Sloppy solve on ensemble 17 on 1024 BC1 cores	0.21 hours
Exact solve on ensemble 17 on 1024 BC1 cores	1.13 hours
Number of configurations	50
Number of sloppy solves per configuration	512
Number of exact solves per configuration	16
Number of Lanczos invocations (different twists) per configuration	8
Total computational cost in Mio Jpsi-core hours	27.3
Total storage on disk	17 TB
Total storage on tape	806 TB
Total storage cost in Mio Jpsi-core hours	2.8
Total request	30.1 Mio Jpsi-core hours

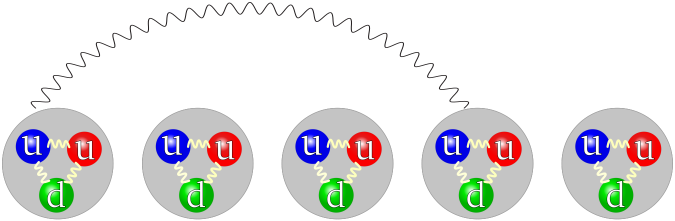
Table 1: Cost estimates for the proposed computation. We intend to use an AMA [6] setup with parameters described in this table.

Bloch's theorem and QCD+QED simulations

arXiv:1503.04395



$\Updownarrow$



Bloch's theorem: a quick reminder

Eigenfunctions of the SE can be written as

$$\psi_{m,n,\theta}(x) = e^{i(2\pi m+\theta)x/L} u_{m,n,\theta}(x)$$

with $u_{m,n,\theta}(x+L) = u_{m,n,\theta}(x)$ and m, n, θ enumerating the states.

Let's consider a single fundamental cell with twisted boundary conditions (and twist-angle θ). We can decompose an arbitrary wavefunction $\phi_\theta(x)$ as

$$\phi_\theta(x) = \sum_{m,n} \psi_{m,n,\theta}(x) c_{m,n}\,.$$

The same wavefunction extended beyond the fundamental cell is then given by

$$\phi(x) = \sum_{m,n} \int_0^{2\pi} d\theta \psi_{m,n,\theta}(x) c_{m,n} = \int_0^{2\pi} d\theta \phi_\theta(x)\,.$$

Prescription for any observable:

1. Before performing the fermionic Wick contractions, replace $\psi \to \Psi$
2. Perform Wick contractions
3. Use Eq. (1) to relate expression back to integrals over twists involving only Dirac inversions of your finite-volume theory

Remarks:

- Allows for the coupling of photons to Ψ and therefore to simulate finite-volume (FV) QCD + infinite-volume QED
- Discrete sum versions of Eq. (1) for larger volume instead of infinite-volume are straightforward
- Put sources/sinks anywhere in infinite volume
- In particular with multi-source methods (such as AMA) can get away with single twist per configuration and source

Brief history of similar ideas:

- PBC+ABC trick
- Metallic systems:
  - arXiv:cond-mat/0101339): "... averaging over the twist results in faster convergence to the thermodynamic limit than periodic boundary conditions ..."
  - Loh and Campbell 1988: "... using a novel phase-randomization technique, we are able to obtain absorption spectra with high resolution"
- Nucleon mass and two-baryon systems (Briceno et al. 2013): "Twist averaging ... improves the volume dependence ..."