Improving the volume-dependence of lattice QCD+QED simulations

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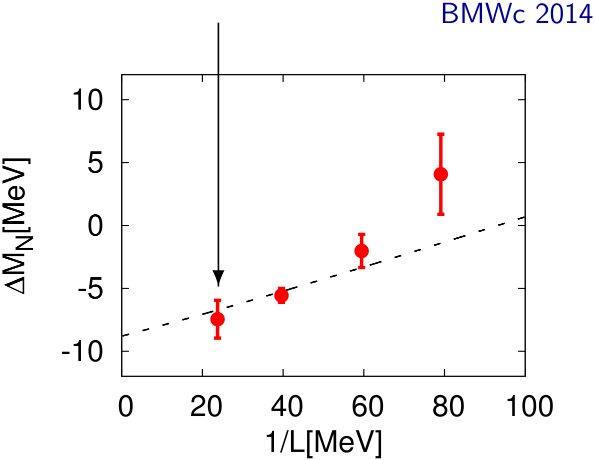
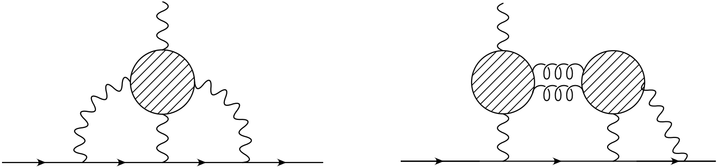
Motivation

$L \approx 9$ fm



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



Unlike the HVP, where we usually treat the QED part in infinite volume analytically and we only compute a QCD form factor (Blum 2000), for the $(g-2)_\mu$ HLbL contribution we compute the full diagram and need to control QED (Luchang's talk).

A selection of studies of interest

Δm_π

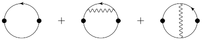


Figure 4: Quark-connected electro-magnetic mass splitting diagrams.

f_π

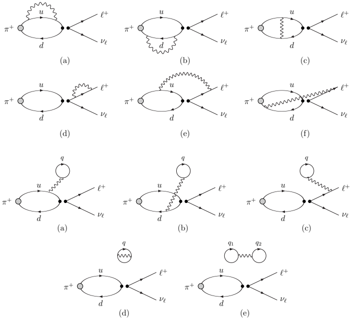


Figure 5: Quark-connected (top) and quark-disconnected (bottom) diagrams for f_π.

$(g-2)_\mu$ HLbL

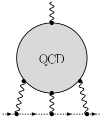


Figure 7: Light-by-light contribution to $(g-2)_\mu$

Carrasco et al. 2015

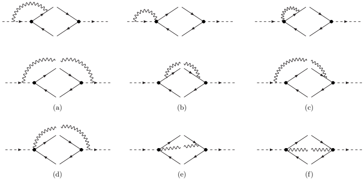


Figure 6: Soft-photon emission in effective field theory.

Target: infinite-volume QCD+QED simulation

Find numerical approximation to infinite-volume QCD+QED with small finite-volume errors

A potential problem: isolated poles turn into cuts and the projection to the ground state may require very large distances.

Assuming the level density $\rho(E)$ is analytic in E, we have

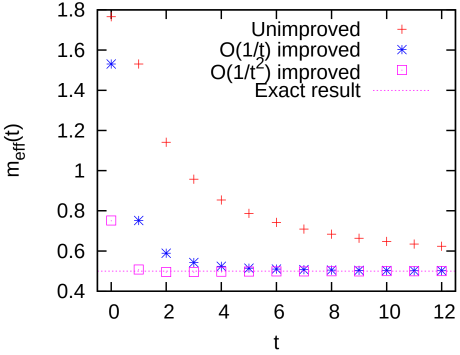
$$C(t) = \int_{E_0}^{\infty} dE\, \rho(E) e^{-Et} = \left(\sum_{m=1}^{\infty} c_m(E_0) t^{-m} \right) e^{-E_0 t}\,, \qquad (1)$$

see backup slides for derivation, and therefore

$$m^{\text{eff}}(t) = E_0 + \sum_{n=1}^{\infty} d_n(E_0) t^{-n}\,. \qquad (2)$$

This extends trivially in the presence of additional isolated poles.

Example: Infinite-volume free Dirac fermion point-source propagator in position space



One possible solution: explicitly cancel the $1/t$ term by defining an improved effective mass

$$m^{\mathrm{eff,O(1/t)}}(t) = (t+1)m^{eff}(t+1) - t\, m^{eff}(t)\,. \tag{3}$$

Introduction to the method

- Extension of twist-averaging procedure: By suitable averages over boundary conditions we can put valence fermions and the coupled photons in infinite volume (for details, please see arXiv:1503.04395). The large/infinite volume can be created in a stochastic manner.

- Here: investigate the role of the QCD and QED part separately.

- Focusing on a single photon propagator $G(x)$, a general QCD-plus-QED diagram can be written as

$$\langle C \rangle = \sum_{x,y} \langle V(x) V(y) O_1(z_1) \dots O_n(z_n) \rangle G(x-y) \,, \tag{4}$$

  where x, y are the fermion-photon vertex positions.

- Cluster decomposition: if we put the operators in Eq. (4) in two groups A and B with A containing $V(x)$ and B containing $V(y)$ and displace the operators A in space-time by Δ, we have for sufficiently large $|\Delta|$

$$\langle A(\Delta)B\rangle - \langle A(\Delta)\rangle\langle B\rangle = 0\,. \tag{5}$$

- Naturally, if for all possible groups $\langle A(\Delta)\rangle\langle B\rangle = 0$, the large distance part of the photon propagator in Eq. (4) is suppressed by the fermionic contractions. In a theory with a mass gap such as QCD, this additional suppression through de-correlation is reached exponentially in $|\Delta|$. We will refer to such cases as *class A* problems. Typical examples are discussed below in the context of QED mass splittings.

- All diagrams not in *class A* will be referred to as *class B*. The connected $(g-2)_\mu$ HLbL diagram falls into this category.

Since the QCD part does in general not have power-like FV errors (such cases require a separate discussion), there are only two sources of power-like FV errors:

1. $1/L^n$ corrections in short-distance part of photon propagator and
2. $1/L^n$ corrections introduced by cutting the long-distance $1/r^2$ photon propagator at the boundary of the simulation volume.

For *class A*, 2) is irrelevant and hence we suggest that for *class A* problems removing $1/L^n$ corrections from the short-distance part of the photon propagator removes power-like finite-volume errors!

For *class B* problems the long-distance part of the photon propagator is crucial. We will discuss a possible solution in the case of $(g-2)_\mu$ below.

In addition to the common QED_L ($\vec{k} = 0$ subtraction) and QED_{TL} ($k = 0$ subtraction), we define QED_∞ through

$$G(x) = \int_{-\pi}^{\pi} \frac{d^4 k}{(2\pi)^4} \frac{e^{ikx}}{\hat{k}^2} \tag{6}$$

with

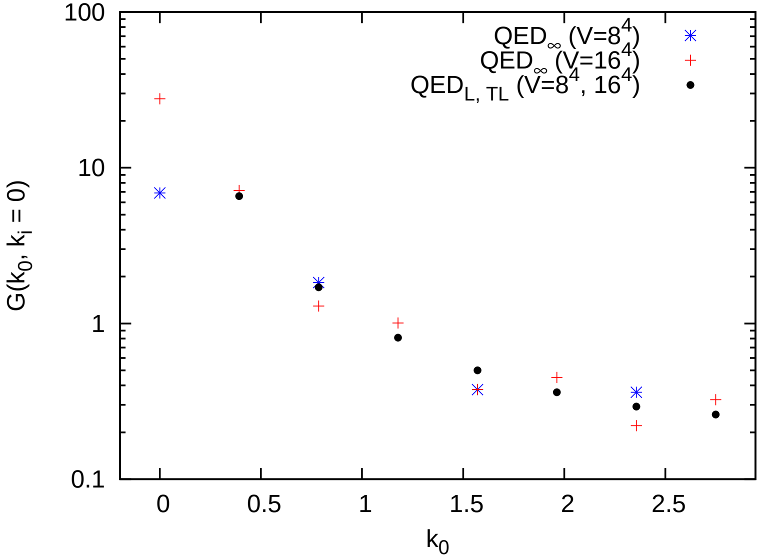
$$\hat{k}_\mu = 2\sin(k_\mu/2) \tag{7}$$

and

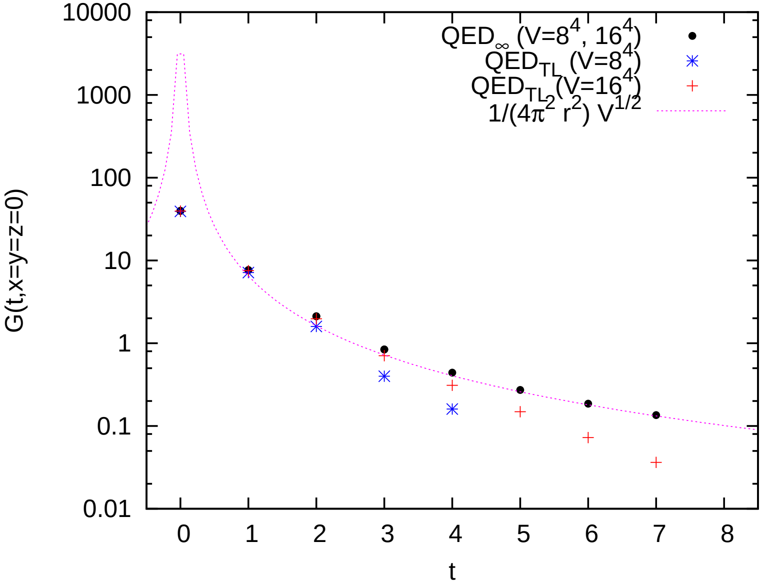
$$\hat{k}^2 = \sum_\mu \hat{k}_\mu^2 \,. \tag{8}$$

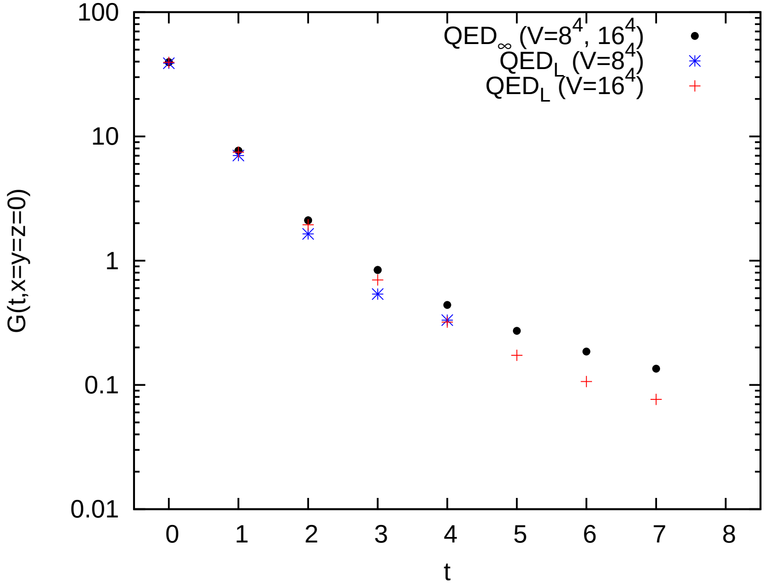
Analytic and numerical methods for an efficient computation are available (Izubuchi, Jin, and C.L. 2015).

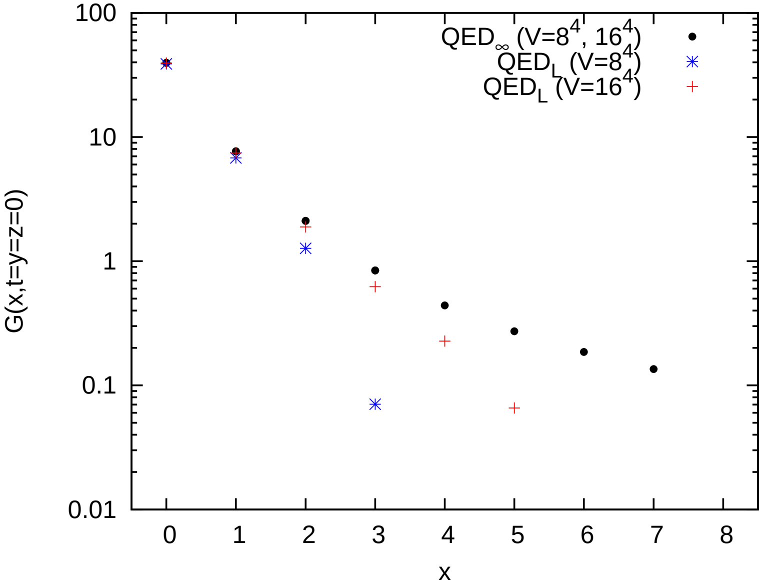
One can use QED_∞ also in dynamical QCD+QED. To this end a simple DFT of $G(x)$ with x in a finite volume yields $G(k)$.



100
10
1
0.1
0
0.5
1
1.5
2
2.5
k_0
$G(k_0, k_i = 0)$
QED_∞ ($V=8^4$)
QED_∞ ($V=16^4$)
$\mathrm{QED}_{L,\,TL}$ ($V=8^4$, 16^4)


QED$_\infty$ (V=8^4, 16^4)
QED$_{TL}$ (V=8^4)
QED$_{TL_2}$(V=16^4)
$1/(4\pi^2 r^2)$ $V^{1/2}$
G(t,x=y=z=0)
t
10000
1000
100
10
1
0.1
0.01
0
1
2
3
4
5
6
7
8

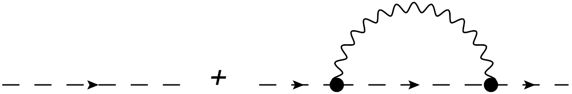

QED$_\infty$ (V=8^4, 16^4)
QED$_L$ (V=8^4)
QED$_L$ (V=16^4)
G(t,x=y=z=0)
t
100
10
1
0.1
0.01
0
1
2
3
4
5
6
7
8



100
10
1
0.1
0.01
G(x,t=y=z=0)
0
1
2
3
4
5
6
7
8
x
QED$_\infty$ (V=8^4, 16^4)
QED$_L$ (V=8^4)
QED$_L$ (V=16^4)

A scalar test

Example: QED mass correction on a lattice in finite volume



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

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

The expected structure of the correlation function is

$$C(t) = C^{(0)}(t) + \alpha^{\mathrm{QED}} C^{(1)}(t) \tag{9}$$

with

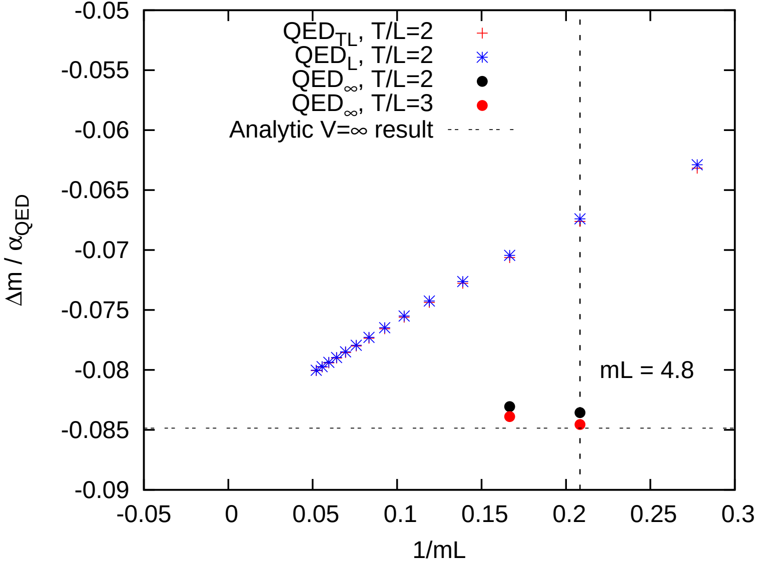
$$C^{(1)}(t) = (\Delta Z^{(1)} - \Delta m^{(1)} t) C^{(0)}(t) \tag{10}$$

such that

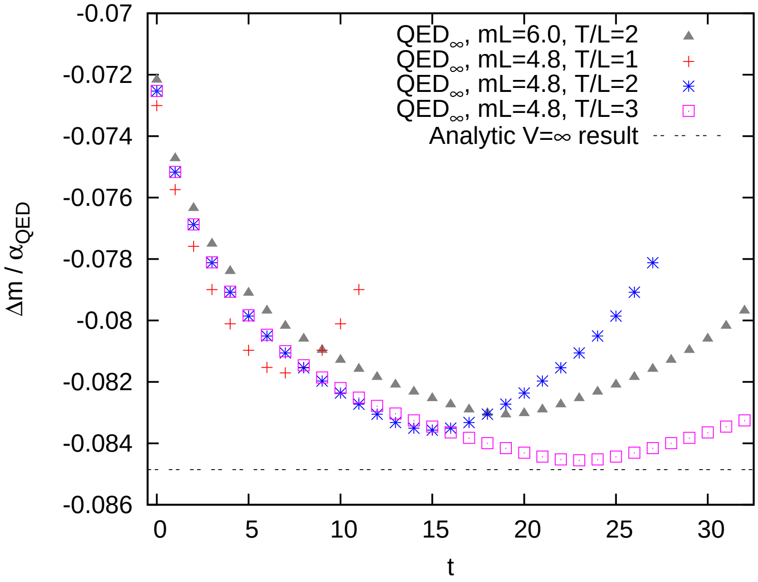
$$C(t) = (1 + \alpha^{\mathrm{QED}} \Delta Z^{(1)}) e^{-\alpha^{\mathrm{QED}} \Delta m^{(1)} t} C^{(0)}(t)\,. \tag{11}$$

We extract

$$\Delta m^{(1)}(t) = \frac{C^{(1)}(t)}{C^{(0)}(t)} - \frac{C^{(1)}(t+1)}{C^{(0)}(t+1)}\,. \tag{12}$$



-0.05
-0.055
-0.06
-0.065
-0.07
-0.075
-0.08
-0.085
-0.09
-0.05
0
0.05
0.1
0.15
0.2
0.25
0.3
Δm / α_QED
1/mL
QED_TL, T/L=2
QED_L, T/L=2
QED_∞, T/L=2
QED_∞, T/L=3
Analytic V=∞ result
mL = 4.8

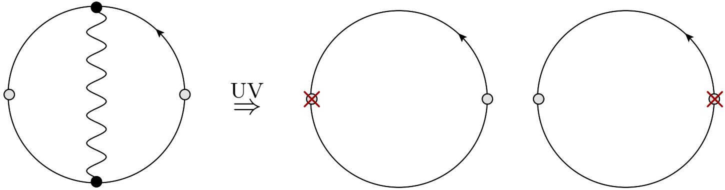


QED$_\infty$, mL=6.0, T/L=2
QED$_\infty$, mL=4.8, T/L=1
QED$_\infty$, mL=4.8, T/L=2
QED$_\infty$, mL=4.8, T/L=3
Analytic V=∞ result
$\Delta m / \alpha_{QED}$
t
-0.07
-0.072
-0.074
-0.076
-0.078
-0.08
-0.082
-0.084
-0.086
0
5
10
15
20
25
30

Δm^{QED} in QCD

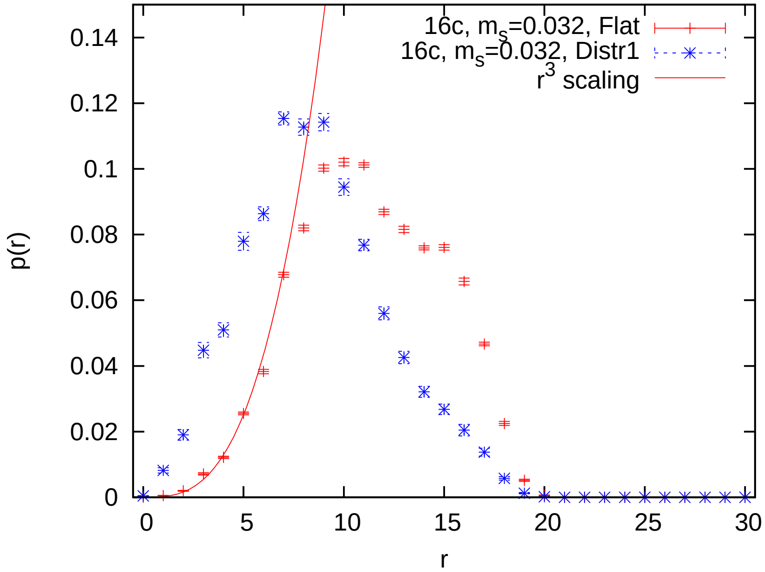
QCD+QED test computation of pion vertex correction diagram

Compute the diagram

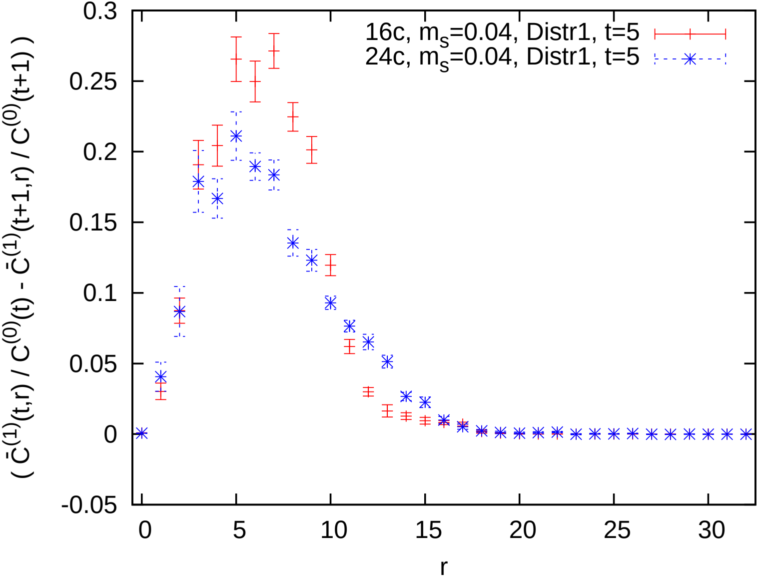


with two local vector currents for now. Ultraviolet part of diagram for finite separation of pions amounts to pion operator renormalization and should not affect the mass splitting.

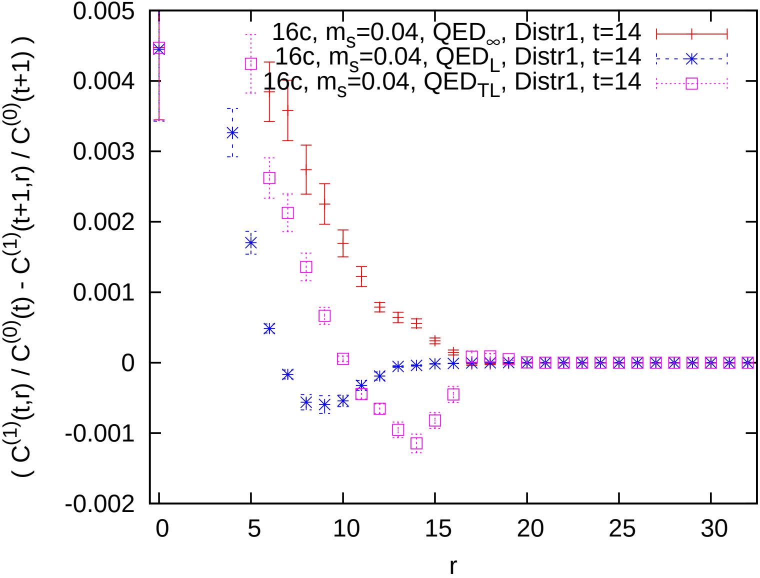
Simulation details: $a^{-1} = 1.73$ GeV, $V = 16^3 \times 32$ and $24^3 \times 64$, $m_\pi = 422$ MeV, 2+1 DWF sea quarks, 20 configurations, 100 point-sources per configuration sampling quark-photon vertex positions; use importance sampling (see Luchang's talk)



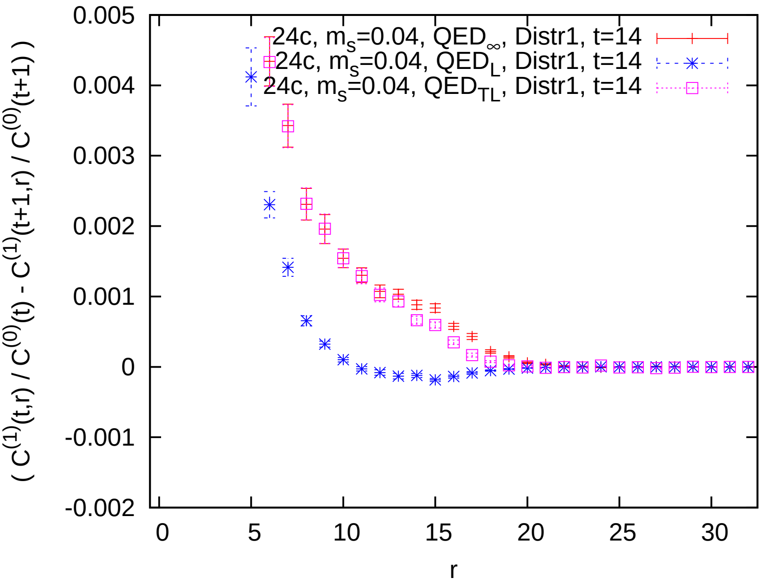
Distribution of distance between sampled quark-photon vertex positions



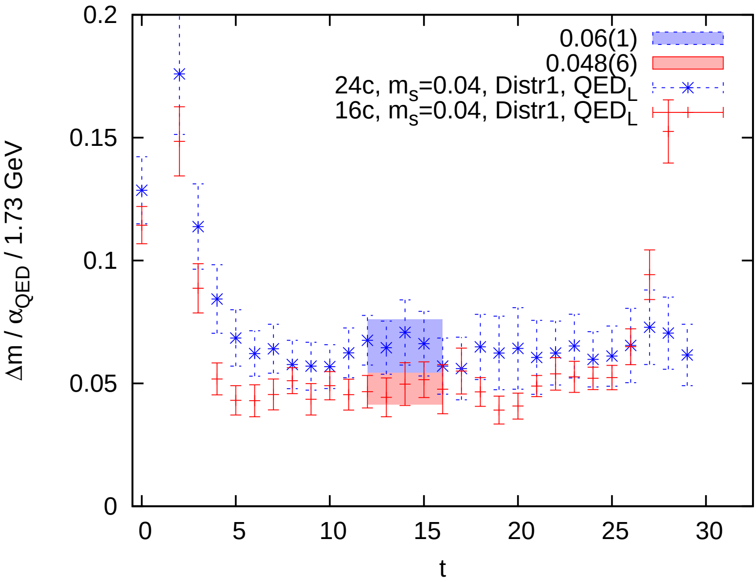
QCD contribution (set $G = 1$) to Δm for photon distance r. TA for valence fermions?



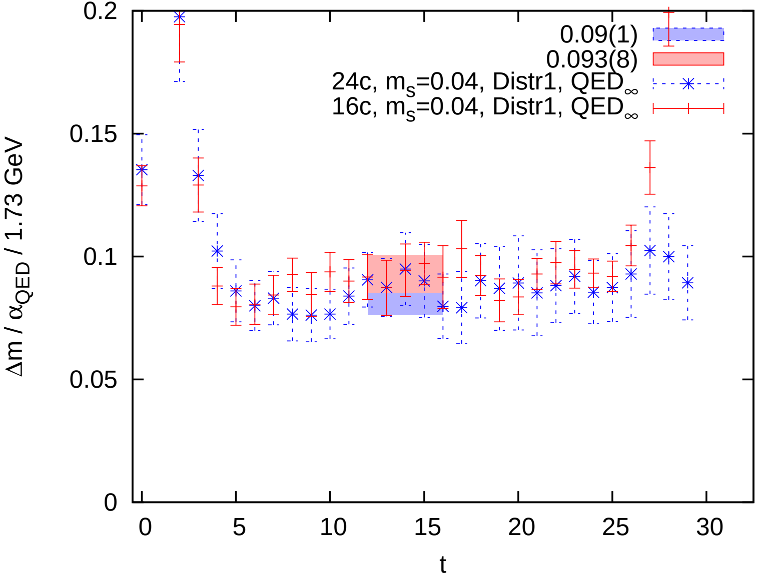
Full Δm for photon distance r. Zero-mode subtraction forces QED_L and QED_{TL} propagators to become negative at large distance. QED_∞ shows little difference between 16^3 and 24^3.

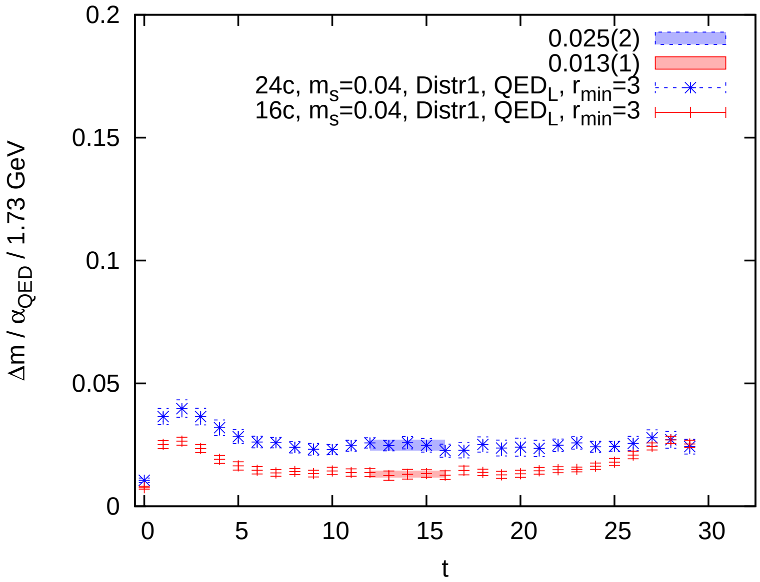


Full Δm for photon distance r. Zero-mode subtraction forces QED_L and QED_{TL} propagators to become negative at large distance. QED_∞ shows little difference between 16^3 and 24^3.

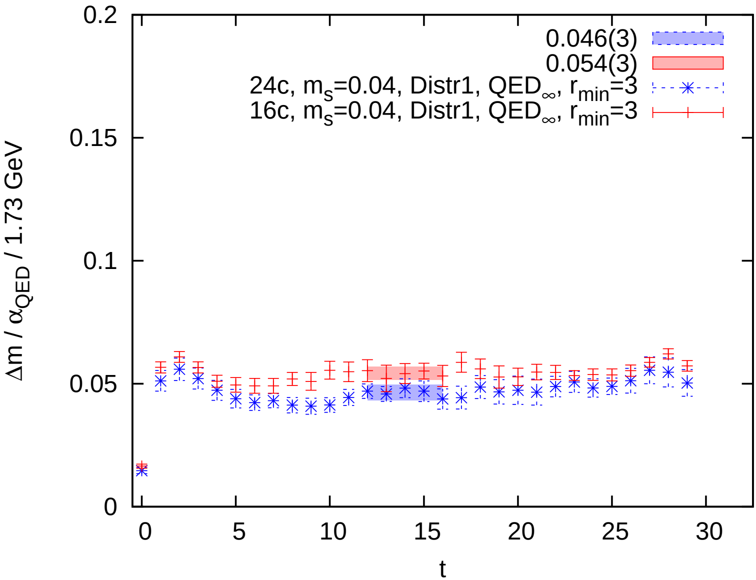


0.06(1)
0.048(6)
24c, m_s=0.04, Distr1, QED_L
16c, m_s=0.04, Distr1, QED_L
$\Delta m / \alpha_{QED}$ / 1.73 GeV
t
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30

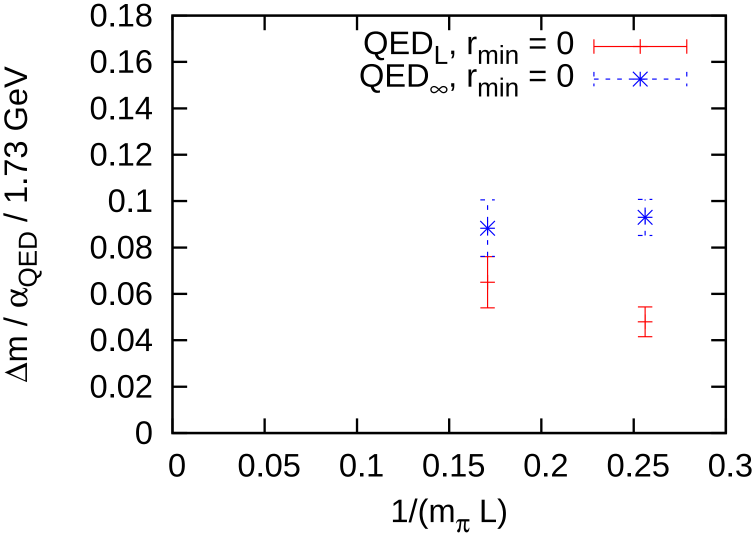

0.09(1)
0.093(8)
24c, m_s=0.04, Distr1, QED_∞
16c, m_s=0.04, Distr1, QED_∞
$\Delta m / \alpha_{QED}$ / 1.73 GeV
t
0
0.05
0.1
0.15
0.2
0
5
10
15
20
25
30



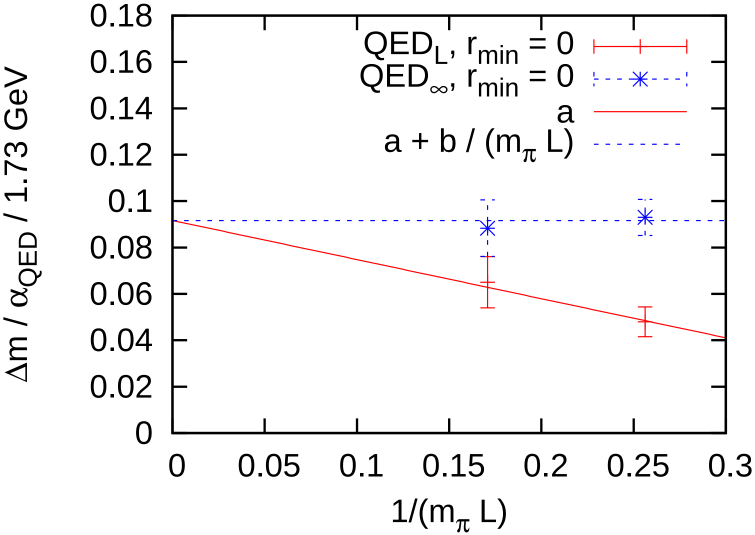
Exclude contributions for $r < r_{\min}$



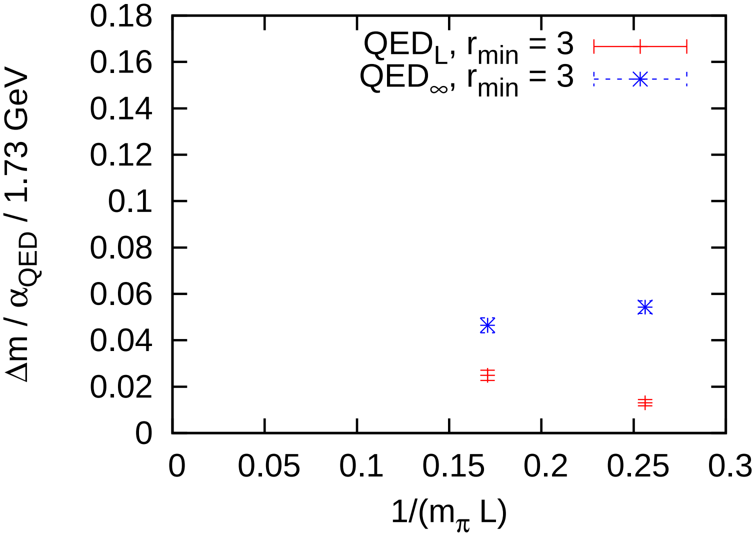
Exclude contributions for $r < r_{\min}$



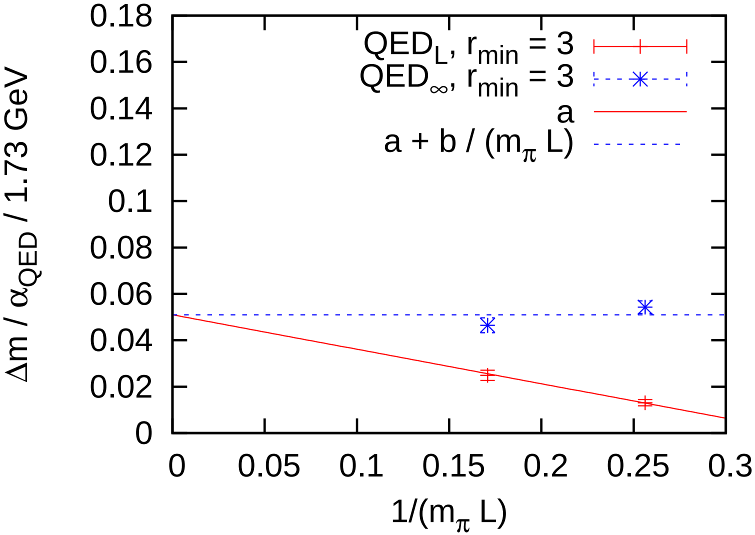
QED_L, r_{min} = 0
QED_∞, r_{min} = 0
$\Delta m / \alpha_{QED}$ / 1.73 GeV
$1/(m_\pi L)$
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.05
0.1
0.15
0.2
0.25
0.3



$\Delta m / \alpha_{QED}$ / 1.73 GeV
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
QED_L, r_{min} = 0
QED_∞, r_{min} = 0
a
a + b / (m_π L)
0
0.05
0.1
0.15
0.2
0.25
0.3
1/(m_π L)

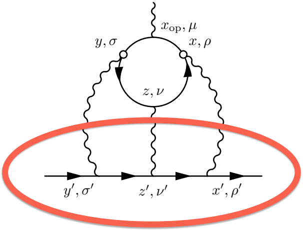


FV behavior largely independent of UV part



FV behavior largely independent of UV part

$(g-2)_\mu$ HLbL

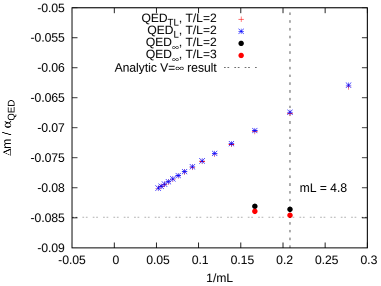


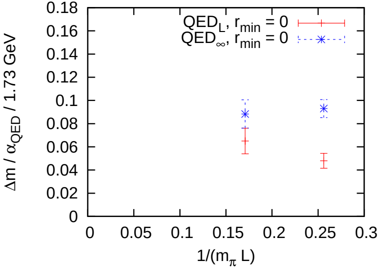
This is a *class B* diagram. After removing the photons, the separate QCD and free muon quantum averages do not vanish and therefore large photon distances are not suppressed. Need to sum over all displacements between QCD and QED part to control FV errors.

Base on method presented in Luchang's talk, compute $M_{\mathcal{A}}^{\mu\nu\rho}(x,y,z) = \sum_{x',y',z'\in\mathcal{A}} G(x'-x)G(y'-y)G(z'-z)\Big[F(x_0-x')\gamma_\mu F(x'-z')\gamma_\rho F(z'-y')\gamma_\nu F(y'-x_1)\Big]$ with $\mathcal{A} = \{(x,y,z,t)|x\in\{-L_x/2,\ldots,L_x/2-1\}, y\in\ldots\}$. Computation for fixed x, y and all z with convolutions has $\mathcal{O}(V\log V)$ cost.

Proposal: Use continuum propagators and vertices and $\sum_{x'\in\mathcal{A}} f(x') \to \int_0^a d\delta^4 \sum_n \sum_{x'\in\mathcal{A}} f(x'+\delta+nL)$ with integral over δ and sum over n stochastically. Work in progress ...

Conclusions





- Discuss and categorize QCD+QED finite-volume errors, introduce QED$_\infty$
- To be published soon
- Outlook: self-energy diagrams, statistics, dynamical QCD+QED, decay constants, complete $(g-2)_\mu$ HLbL infinite-volume study

Backup

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 $\hat{L}_1=(L_1,0)$, $\hat{L}_2=(0,L_2)$

arXiv:1503.04395

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

$$\boxed{\left\langle \Psi_{x+nL}\bar{\Psi}_{y+mL}\right\rangle = \int_0^{2\pi}\frac{d\theta}{2\pi}e^{i\theta(n-m)}\left\langle \psi^\theta_x\bar{\psi}^\theta_y\right\rangle\,, \qquad (13)}$$

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.

Twist-averaged version:

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

Perform sum over m using Poisson's summation formula yields

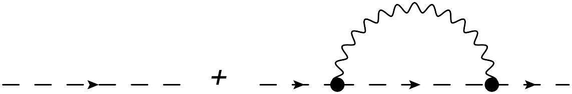
$$
\begin{aligned}
& \sum_m e^{ik(y+mL)} \left\langle \Psi_{x+nL} \bar{\Psi}_{y+mL} \right\rangle \left\langle \Psi_{y+mL} \bar{\Psi}_{z+lL} \right\rangle \\
& = e^{iky} \int_0^{2\pi} \frac{d\theta}{2\pi} \int_0^{2\pi} \frac{d\theta'}{2\pi} e^{i\theta n - i\theta' l} \hat{\delta}(k - (\theta - \theta')/L)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

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



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

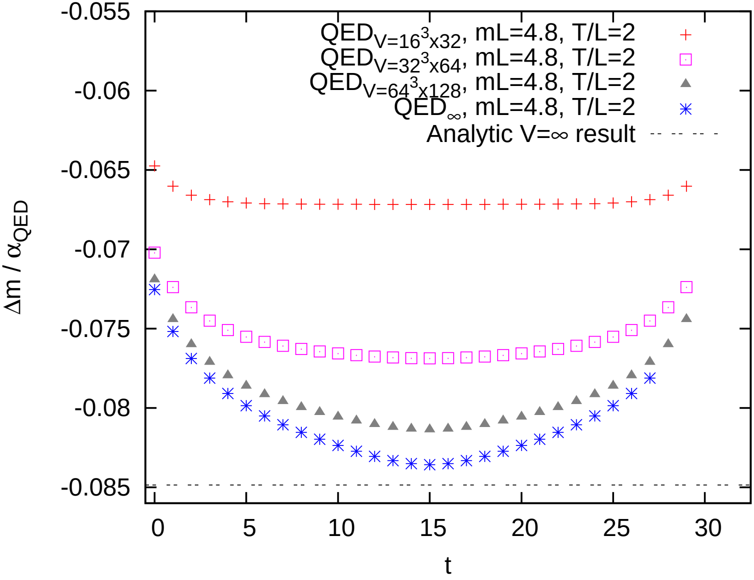
with $\overline{p}_\mu = 2\sin(p_\mu/2)$ and $k'_\mu = k_\mu + \theta_\mu / L_\mu$

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

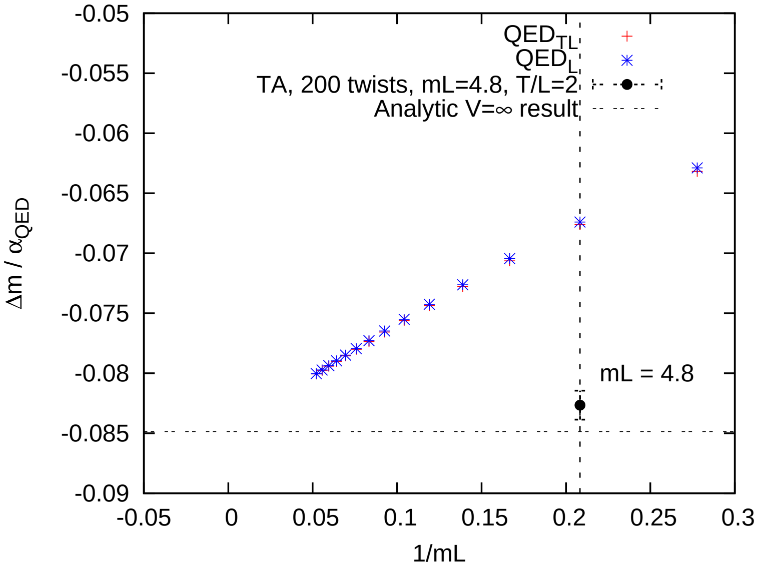
Infinite-volume correlator with dense set of states and analytic $\rho(E)$:

$$
\begin{aligned}
C(t) &= \int_{E_0}^{\infty} dE\; \rho(E) e^{-Et} = \sum_{n=0}^{\infty} b_n \int_{E_0}^{\infty} dE\; E^n e^{-Et} \\
&= \sum_{n=0}^{\infty} b_n (-1)^n \partial_t^n t^{-1} e^{-E_0 t} = \left(\sum_{m=1}^{\infty} c_m(E_0) t^{-m} \right) e^{-E_0 t} \,.
\end{aligned}
\tag{14}
$$

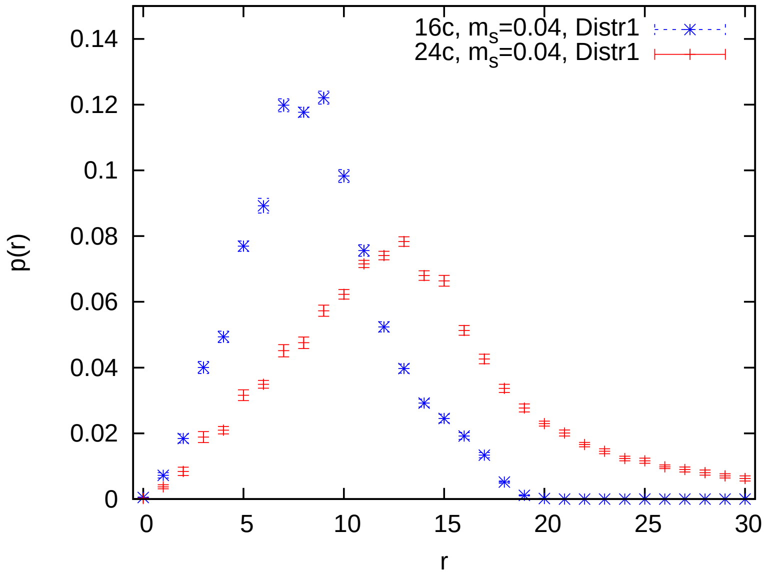
Trivially extended to case of additional isolated poles.



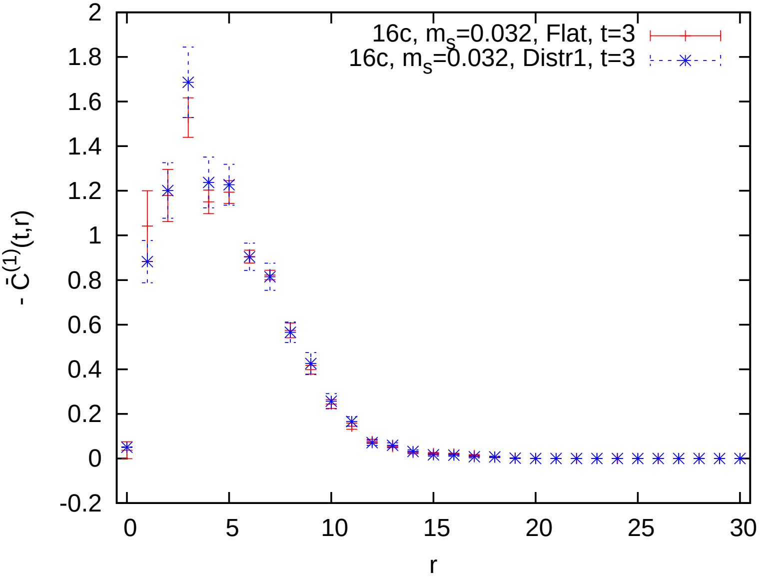
$\mathrm{QED}_{V=16^3x32}$, mL=4.8, T/L=2
$\mathrm{QED}_{V=32^3x64}$, mL=4.8, T/L=2
$\mathrm{QED}_{V=64^3x128}$, mL=4.8, T/L=2
QED_{∞}, mL=4.8, T/L=2
Analytic V=∞ result
$\Delta m / \alpha_{QED}$
t
-0.055
-0.06
-0.065
-0.07
-0.075
-0.08
-0.085
0
5
10
15
20
25
30



QED$_{TL}$
QED$_{L}$
TA, 200 twists, mL=4.8, T/L=2
Analytic V=∞ result
mL = 4.8
-0.05
-0.055
-0.06
-0.065
-0.07
-0.075
-0.08
-0.085
-0.09
$\Delta m / \alpha_{QED}$
-0.05
0
0.05
0.1
0.15
0.2
0.25
0.3
1/mL



16c, m_s=0.04, Distr1
24c, m_s=0.04, Distr1
p(r)
r
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0
5
10
15
20
25
30



16c, m_s=0.032, Flat, t=3
16c, m_s=0.032, Distr1, t=3
$-\bar{C}^{(1)}(t,r)$
r
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
5
10
15
20
25
30