Towards the large volume limit

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arXiv:1406.XXXX

This talk aims to address:

- A specific prescription to put valence fermions and photons in infinite volume
- Applications to the μ–HVP (removal of fit-dependence, study of statistical errors, direct stochastic integration)
- QCD + infinite-volume QED simulations

The setup

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

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

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

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.

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:

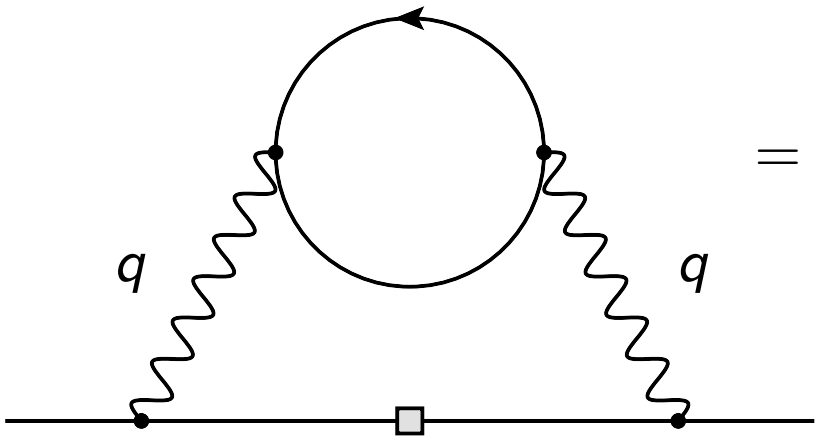
- Allows for the coupling of photons to Ψ and therefore to simulate finite-volume (FV) QCD + infinite-volume QED without power-law FV errors! (More later)
- Discrete sum versions of Eq. (1) for larger volume instead of infinite-volume are straightforward
- Put sources/sinks anywhere in infinite volume
- In particular with multi-source methods (such as AMA) can get away with single twist per configuration and source

Brief history of similar ideas:

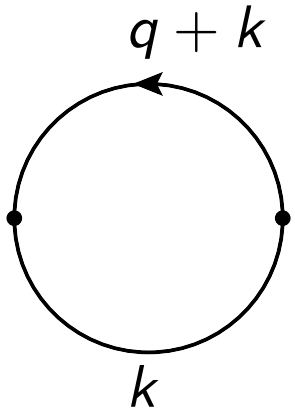
- PBC+ABC trick
- Metallic systems:
  - arXiv:cond-mat/0101339): "... averaging over the twist results in faster convergence to the thermodynamic limit than periodic boundary conditions ..."
  - Loh and Campbell 1988: "... using a novel phase-randomization technique, we are able to obtain absorption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

The muon hadronic vacuum polarization

Blum 2002



$$= \int_0^\infty d(q^2) f(q^2) \left(\frac{1}{q^2} \right.$$

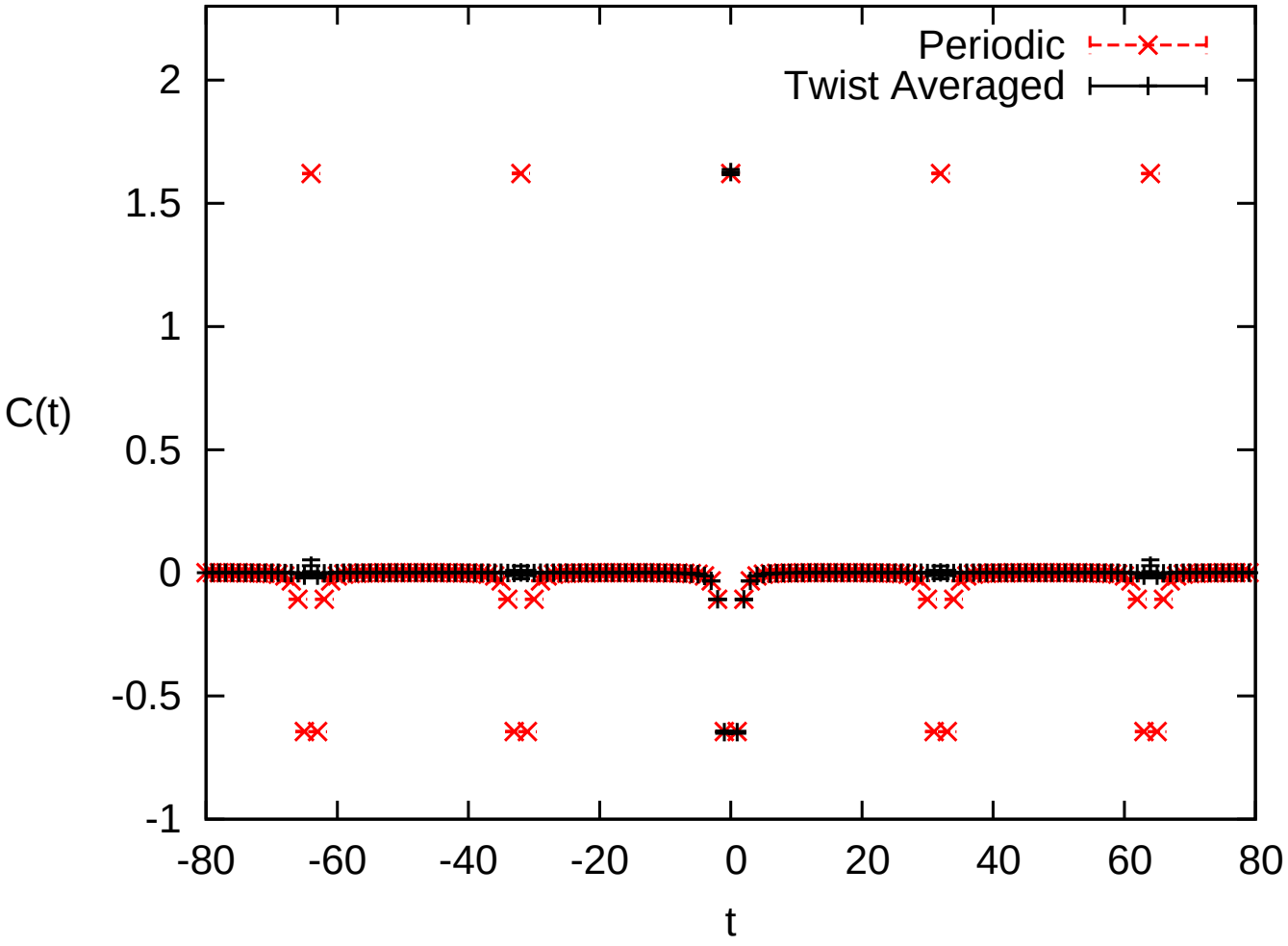


$$\left. -(q \to 0) \right)$$

$$= \hat{\Pi}(q^2)$$

In the following we study this integral with different twist-averaging (TA) methods on RBC/UKQCD's 16^3 and 24^3 ensembles with $a^{-1} \approx 1.73$ GeV and $m_l = 0.01$, $m_s = 0.04$ (and $m_s = 0.032$).

We shall discuss $\Pi_{\mu\nu}(x) = \left\langle V_\mu^{\text{cons.}}(x) V_\nu^{\text{loc.}}(0) \right\rangle$ and define $C_{\mu\nu}(t) = \sum_{\vec{x}} \Pi_{\mu\nu}(x_0 = t, \vec{x})$, $C(t) = C_{\mu\mu}(t)$ for $\mu = 1, 2, 3$.



Problem: noise due to cancellation for small q^2 region

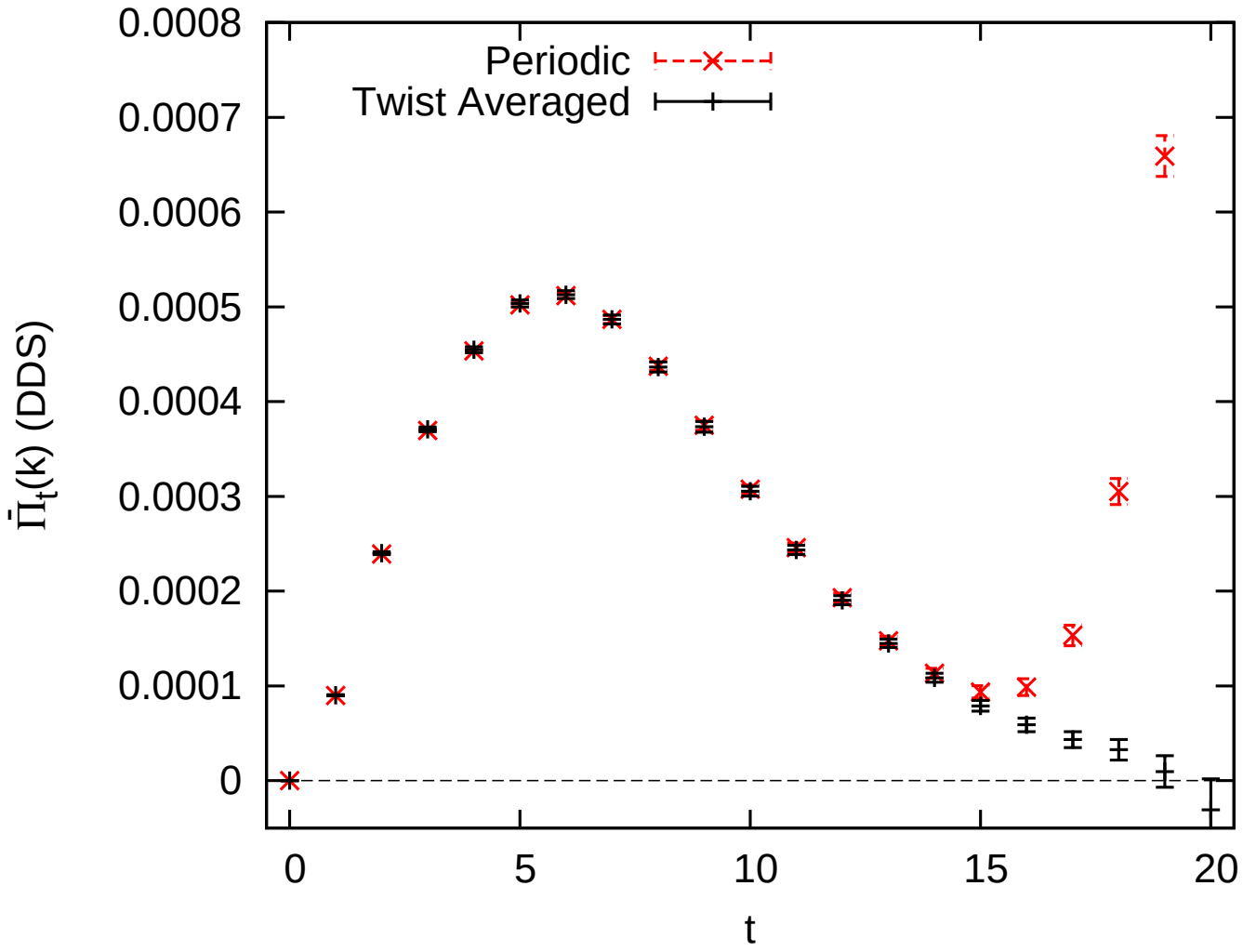
Method 1: Twist-averaged, direct double subtraction:

Origin of noise: Estimators do not satisfy configuration-by-configuration the properties that hold after quantum average such as $\left\langle \Pi_{\mu\nu}(q^2=0)\right\rangle = 0$, $\left\langle \mathrm{Im}\,\Pi_{\mu\nu}(q^2)\right\rangle = 0$.

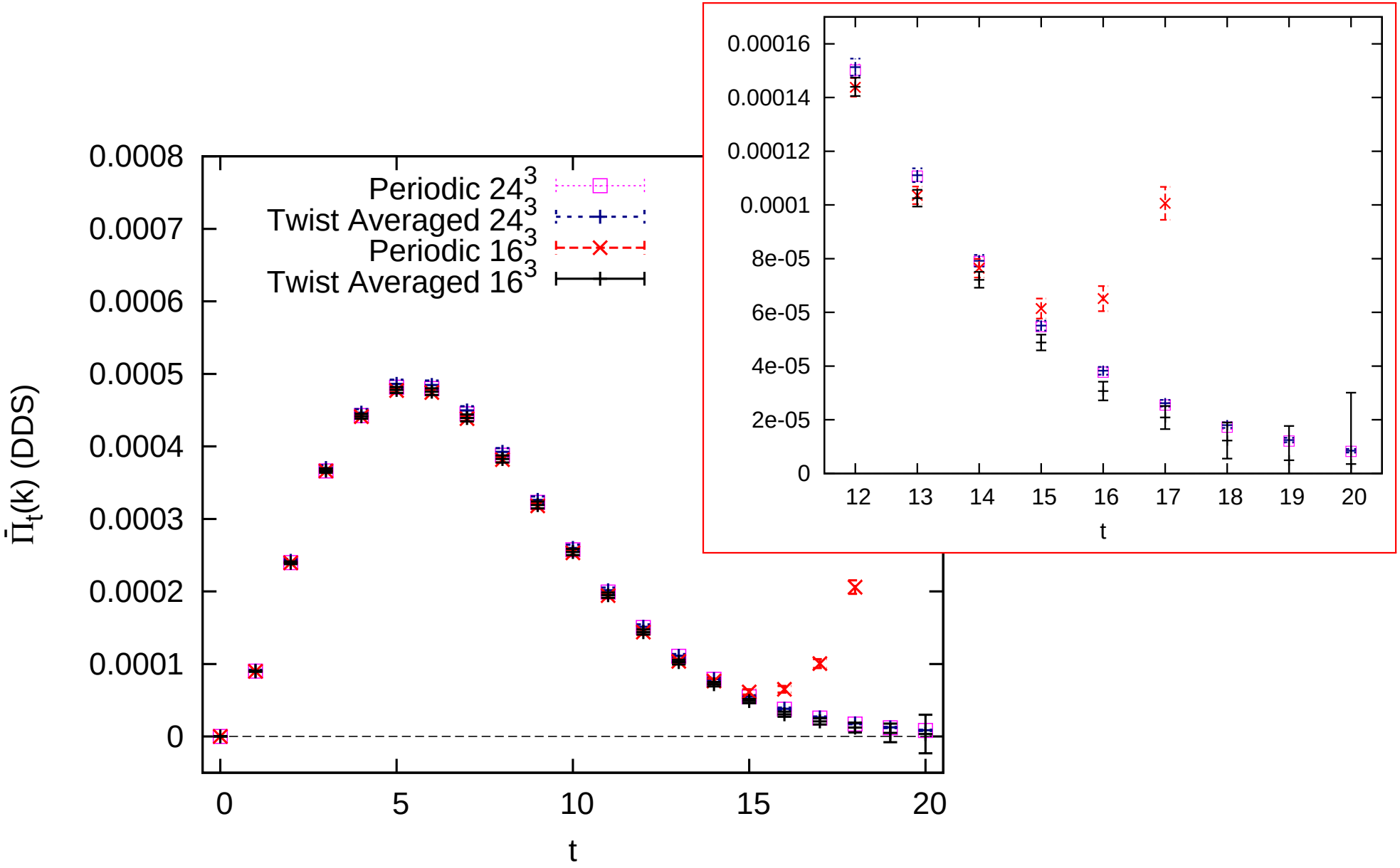
Solution: Estimator that has these properties config-by-config: (Historical: e+e- trick)

$$\left\langle \hat{\Pi}(q^2)\right\rangle = \left\langle \sum_t \mathrm{Re}\left(\frac{exp(iqt)-1}{q^2} + \frac{1}{2}t^2\right)\mathrm{Re}\,C_{\mu\mu}(t)\right\rangle \qquad (2)$$

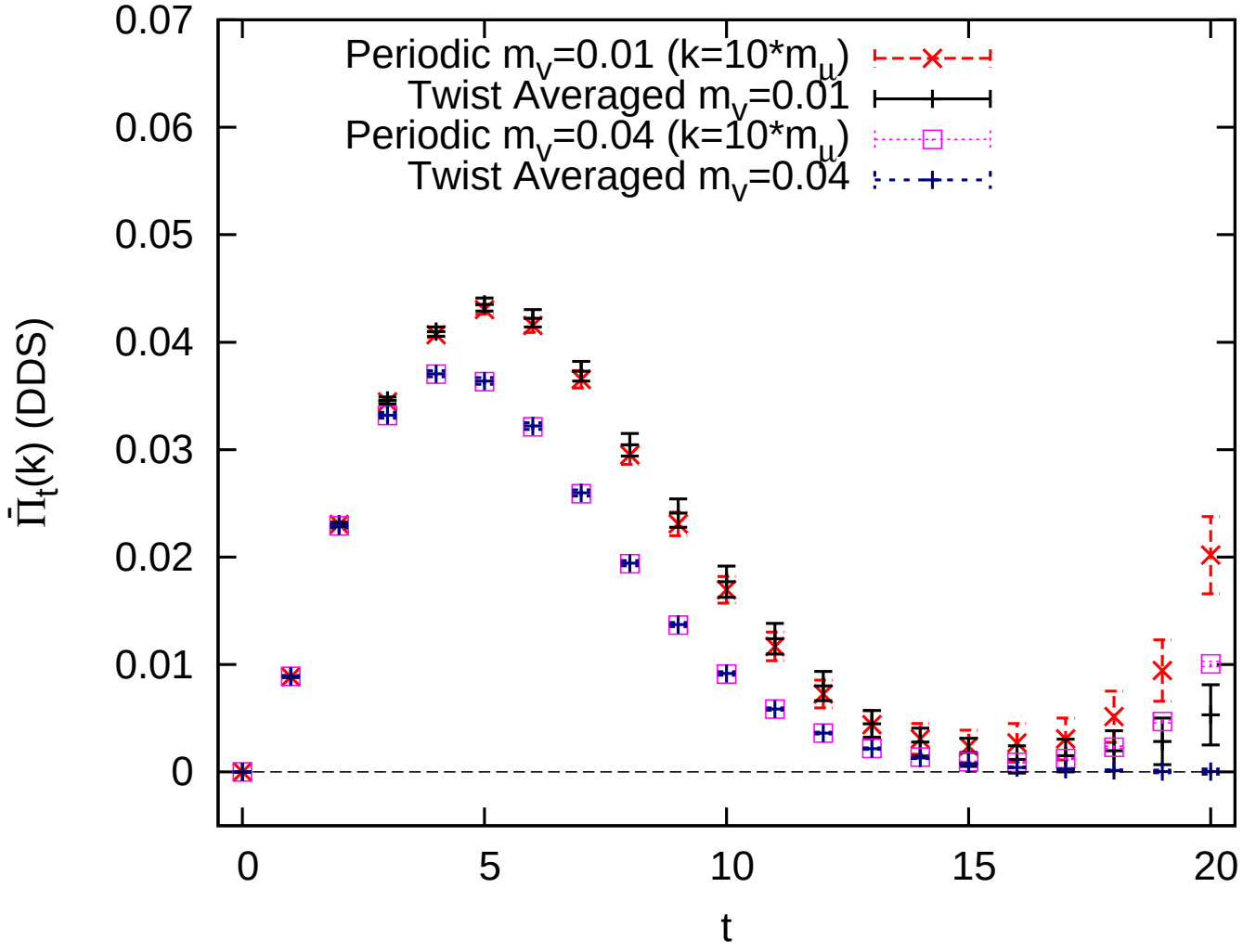
A similar expression can be derived for $\mu \neq \nu$ (arXiv:1406.XXXX)



16^3, $m_v = 0.032$, $k = m_\mu$, ≈ 3000 measurements

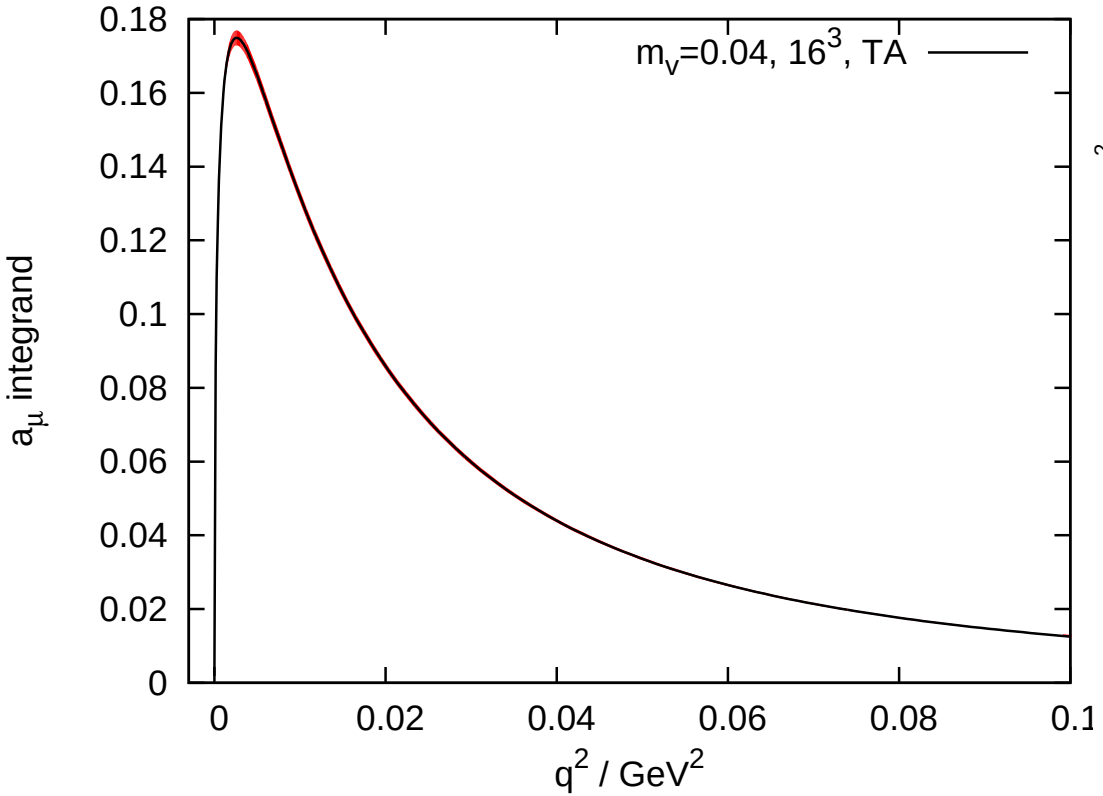


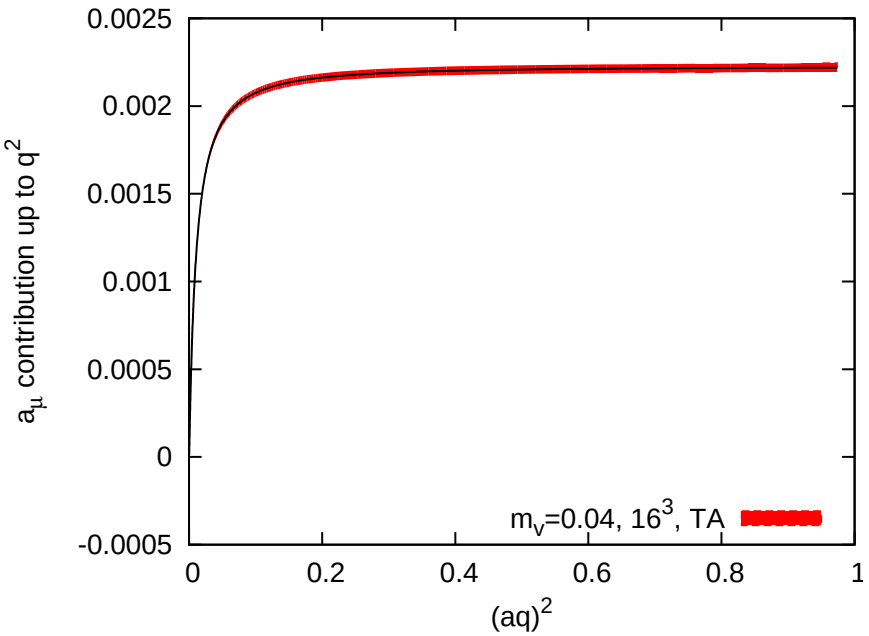
No FV error (sea effects, PQ) resolvable comparing TA 16^3 and 24^3.
In 24^3 periodic and TA identical (within errors) using a cutoff.



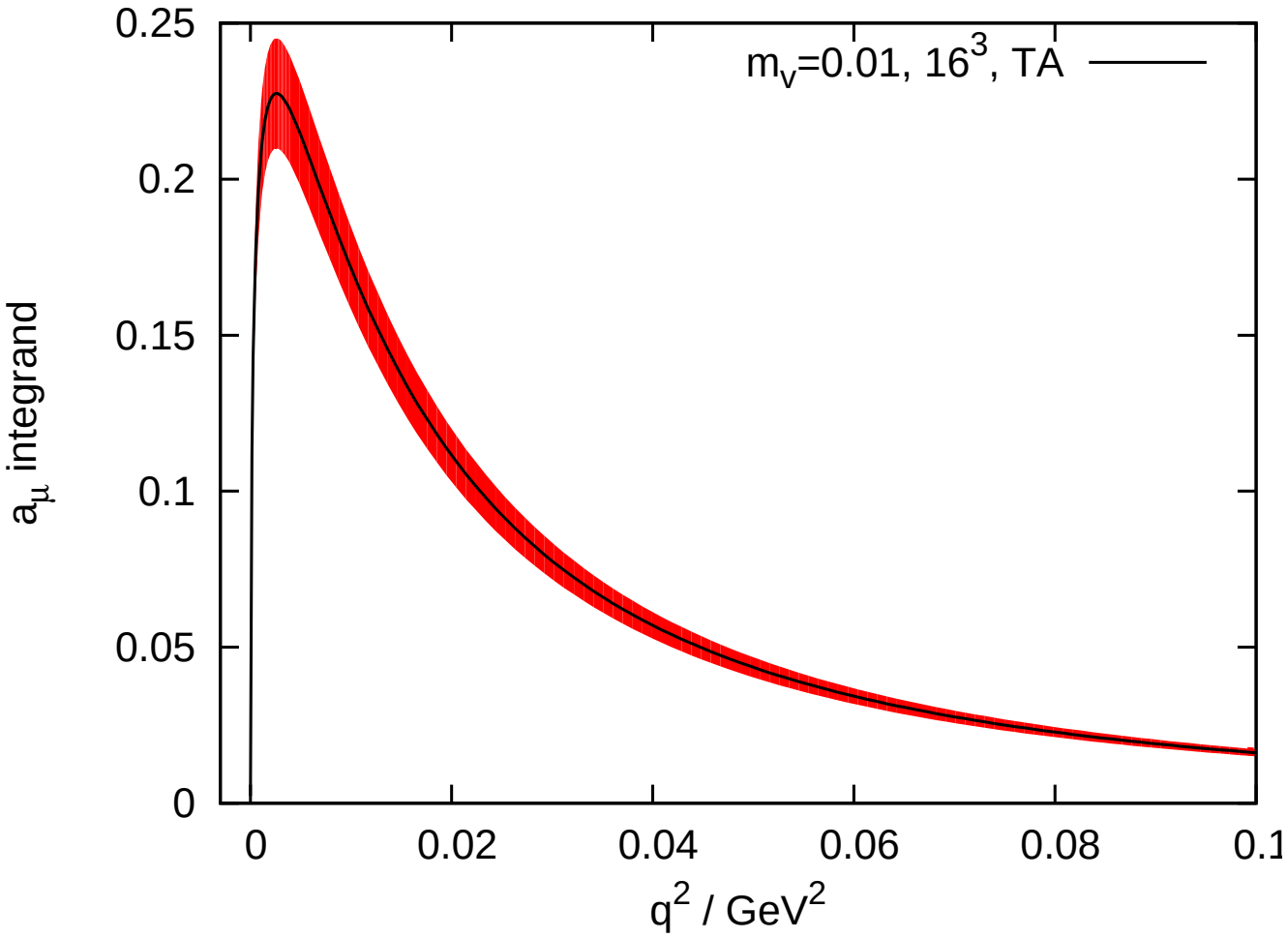
16^3, $m_v = 0.01$ ($m_\pi \approx 422$ MeV), ≈ 120 measurements

See later: deflation

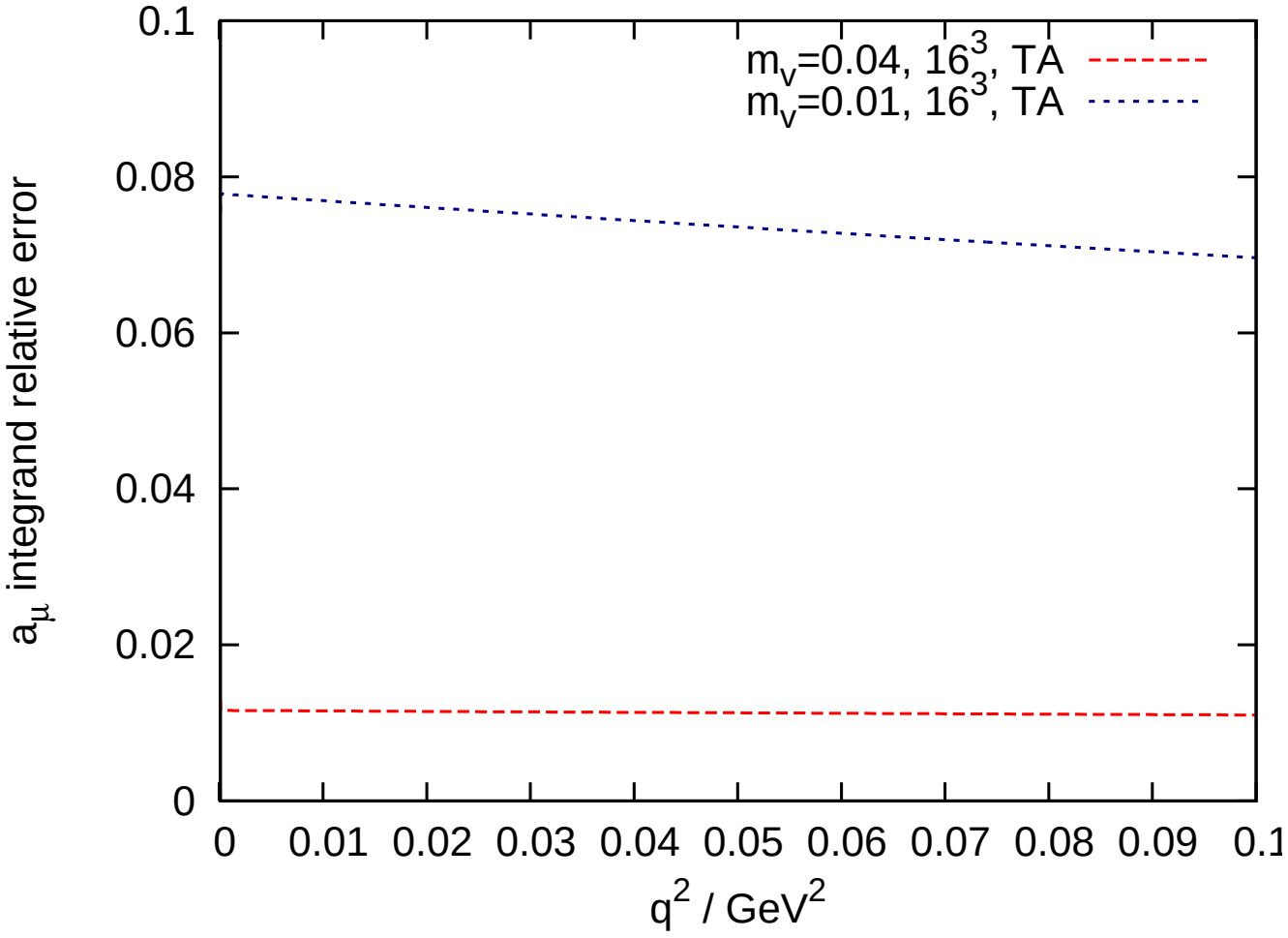




- Arbitrary momentum resolution
- For integral: Trapezoidal / Simpson's rule and use sufficiently fine mesh such that difference is smaller than 1/100 of the statistical error

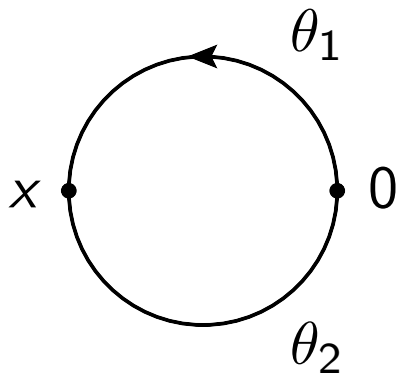


Light quark result with $\approx$ 120 measurements



- After deflation and AMA: same statistics for light quarks as in strange quark case yields $\approx 1/5$ of current light quark error
- For deflation: Peter Boyle's HDCG, chopping up EV to re-use $\theta = 0$ case

Method 2: Direct stochastic integration



Follow the prescription

$$\pi_{\mu\nu}(k) = \int_0^{2\pi} \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi} \sum_{x\in\{0,\dots,L-1\},n\in\mathbb{N}} e^{ik(nL+x)+in(\theta_1-\theta_2)} C_{\mu\nu}(x,\theta_1,\theta_2)$$

and perform sum over n using Poisson's summation formula yields

$$\pi_{\mu\nu}(k) = \int_0^{2\pi} \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi} \sum_{x\in\{0,\dots,L-1\}} e^{ikx}\hat{\delta}(k-(\theta_2-\theta_1)/L) C_{\mu\nu}(x,\theta_1,\theta_2)$$

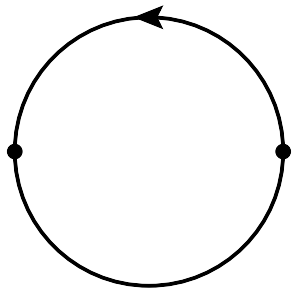
with $\hat{\delta}(k) = \frac{2\pi}{L}\sum_{n\in\mathbb{N}} \delta(k+2\pi n/L)$.

Then: perform k and θ integrals stochastically (use Jacobian to flatten integrand), and use a similar direct double subtraction to reduce noise.

Nice picture in momentum space if we perform one of the θ integrals first:

$$k + q_{\mathrm{PBC}} + \theta_q/L$$

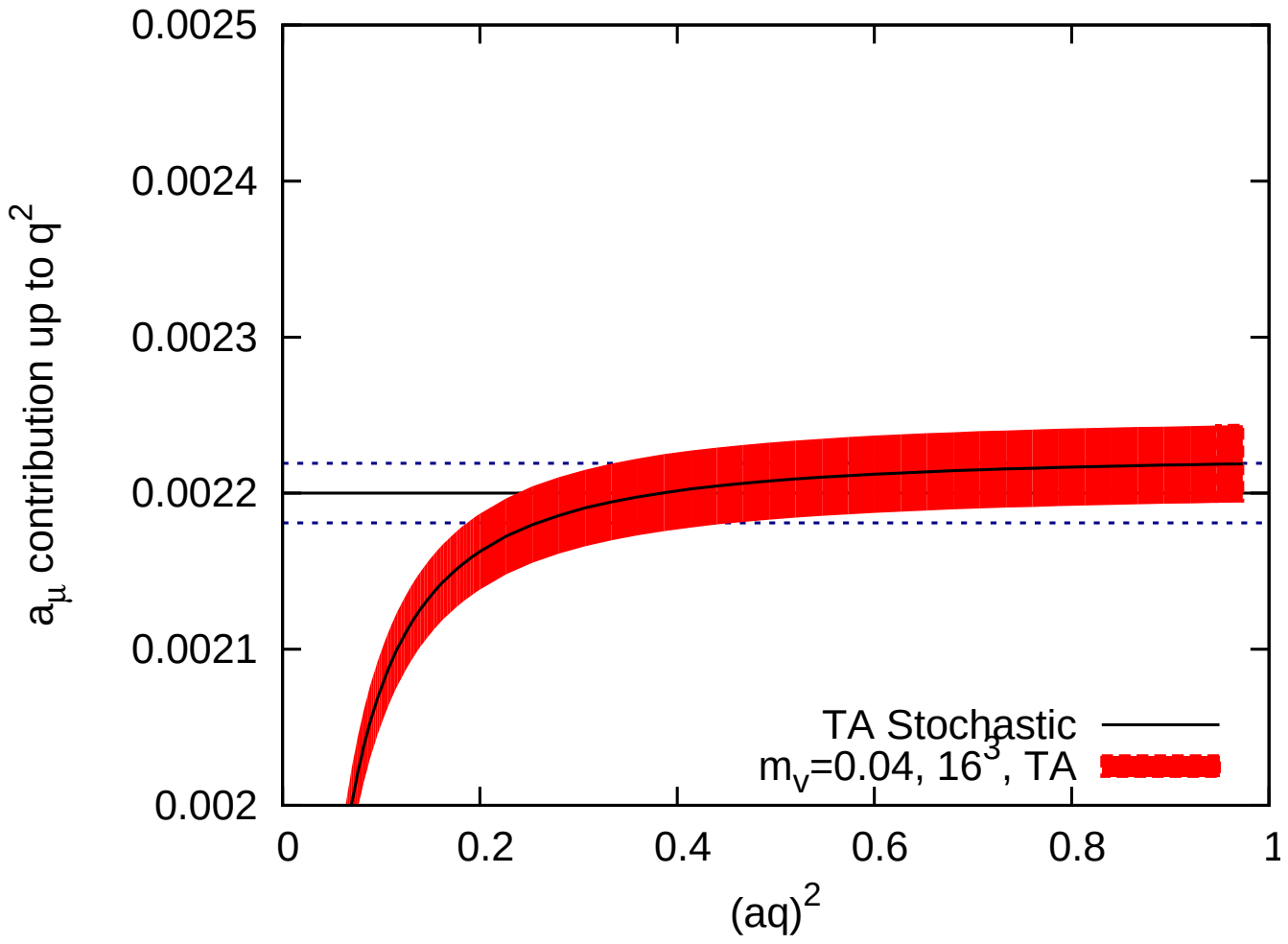
$$\pi_{\mu\nu}(k) = \sum_{q_{\mathrm{PBC}}=\{0,\pm 2\pi/L,\ldots\}} \Big\langle$$

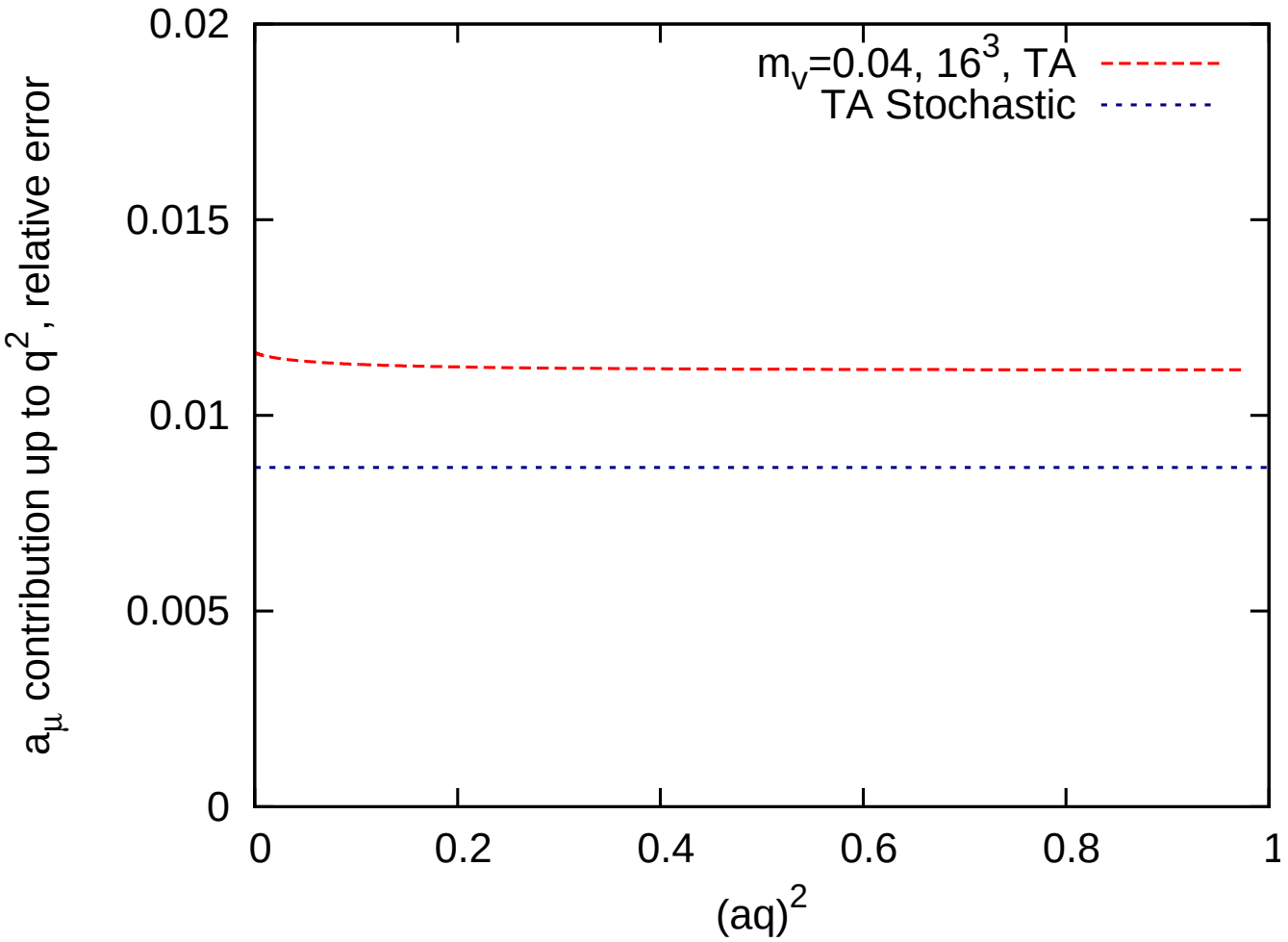


$$\Big\rangle_{\theta_q}$$

$$q_{\mathrm{PBC}} + \theta_q/L$$

However: we perform the k integral first $\Rightarrow$ sampling over θ_1, θ_2 yields a_μ

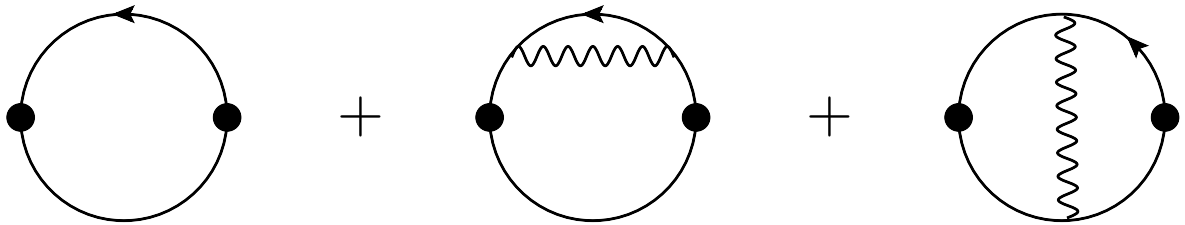

0.0025
0.0024
0.0023
0.0022
0.0021
0.002
0
0.2
0.4
0.6
0.8
1
a_μ contribution up to q^2
$(aq)^2$
TA Stochastic
m_V=0.04, 16^3, TA



Effect of Jacobian?

QCD + QED in infinite volume

Example: QED corrections to effective masses



$$= C_0(t) + \alpha C_1(t)$$

We could compute QED mass-shifts from

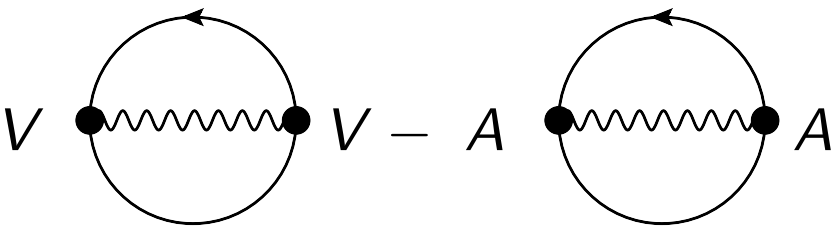
$$m_{\rm eff}(t) = m_{\rm eff,0}(t) + \alpha m_{\rm eff,1}(t)\,, \qquad m_{\rm eff,1}(t) = \frac{C_1(t)}{C_0(t)} - \frac{C_1(t+1)}{C_0(t+1)}\,.$$

Following the prescription and adding $D_G^{\mu\nu}(q^2) = \delta_{\mu\nu}/q^2 + (1-\xi)q_\mu q_\nu/(q^2)^2$ yields photons in infinite volume **and no $1/L^n$ FV effects for QED**.

The setup is similar to the HVP computation discussed above (conserved vector currents yielding a q^2 suppression of the QCD amplitudes) but for the above figure we need four twist angles (per dimension).

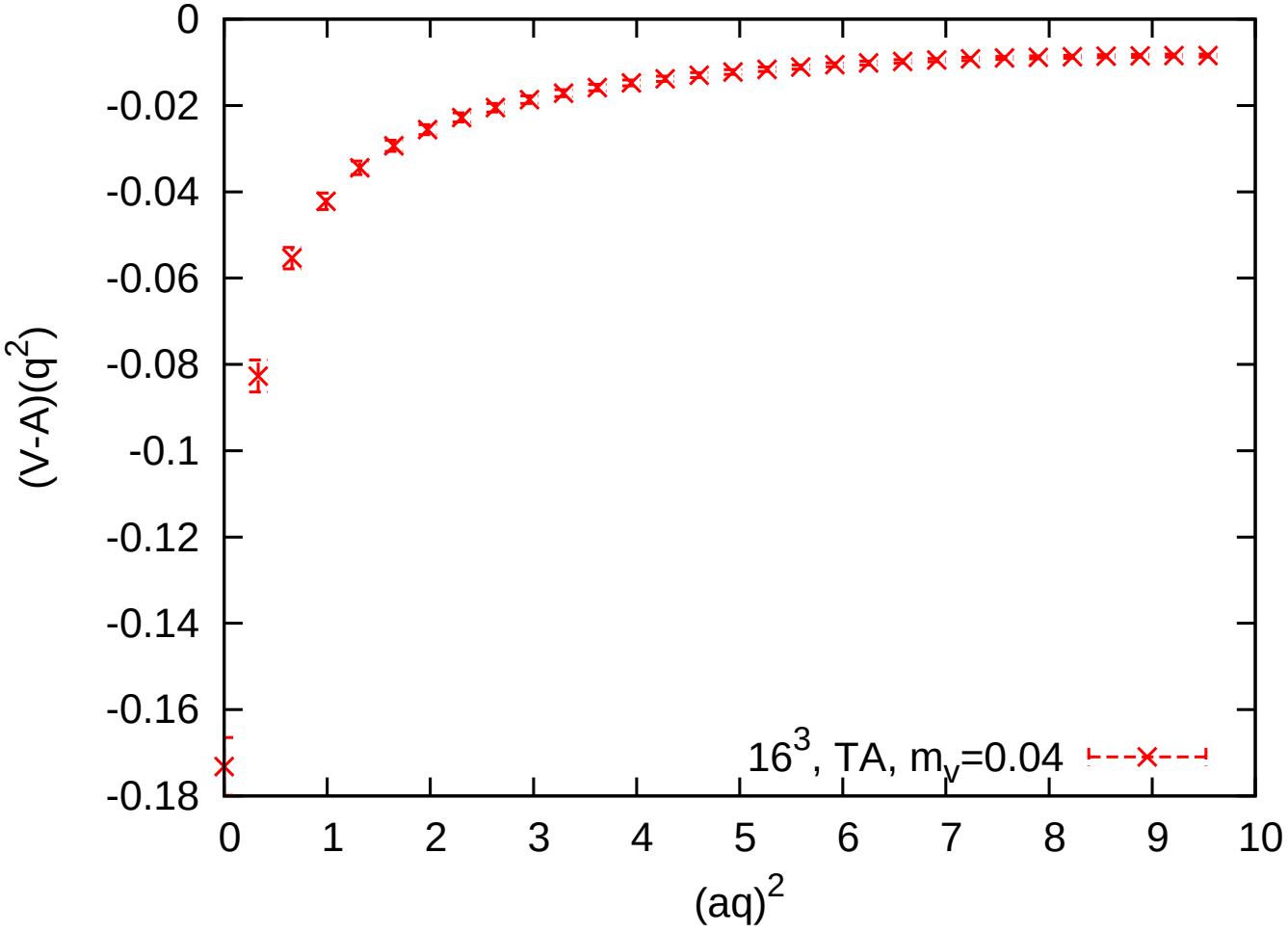
For a first test, we use current algebra and soft pion theorems (Das et al. 1967, Yamawaki 1982, Harada et al. 2004, Shintani et al. 2007)

$\Delta m_\pi^2 =$



This allows us to re-use part of the measurements of the HVP computation for this test.

Integrand with photon momentum q^2:



- Very heavy mass: gap at large q^2 such that integral does not converge
- Stochastic integration of photon momentum ($(aq)^2 < 1$): $-0.095(4)$ ($\approx 4\%$ error)

Conclusion

We have discussed (arXiv:1406.XXXX):

- a prescription for valence fermions and photons in infinite volume (that also works for flavor-diagonal states and allows to put sources/sinks anywhere in the infinite volume)
- two applications to the μ-HVP (connected contribution)
- Finite-volume QCD coupled to infinite-volume QED (no more $1/L^n$ effects)

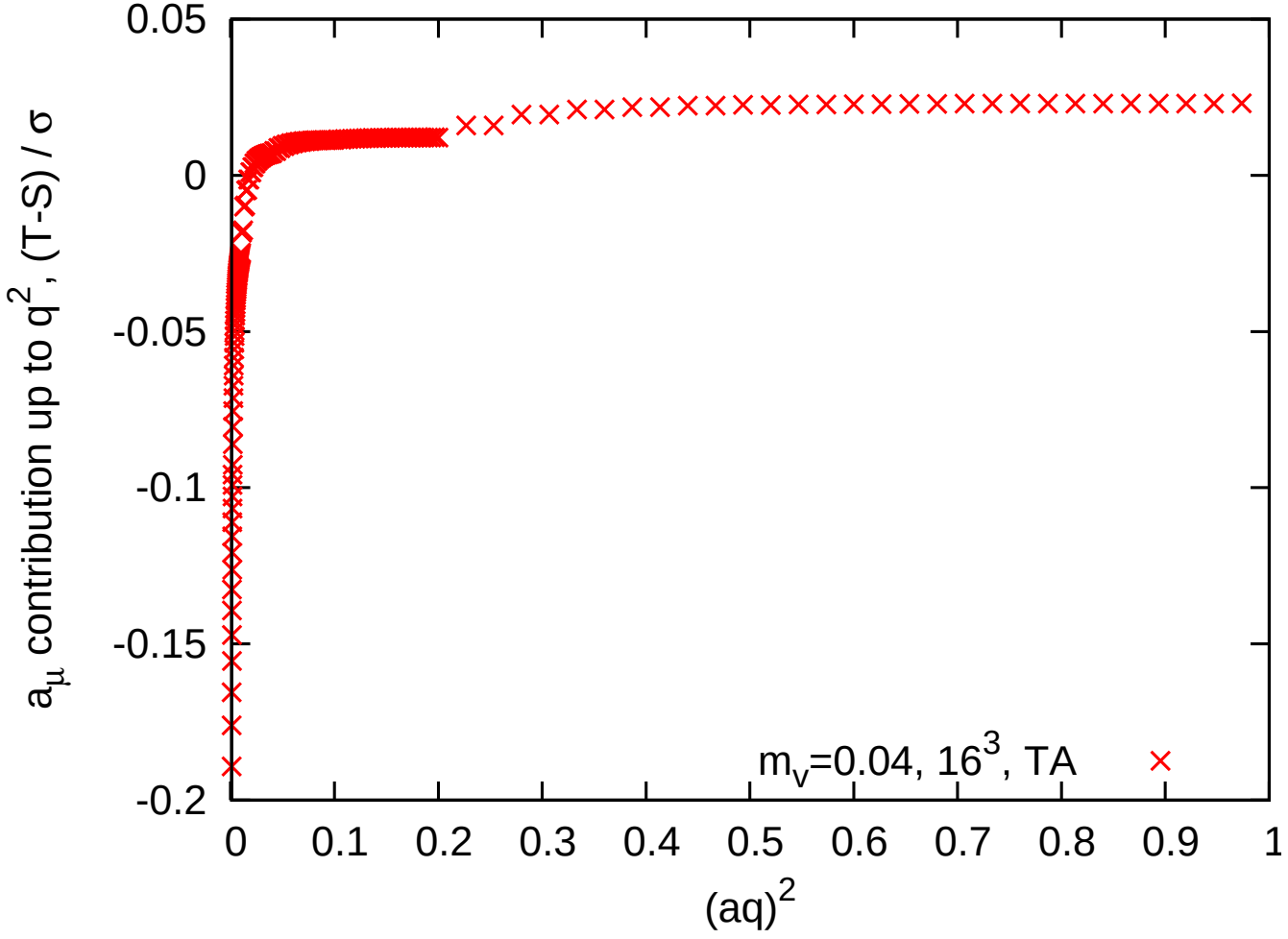
Outlook:

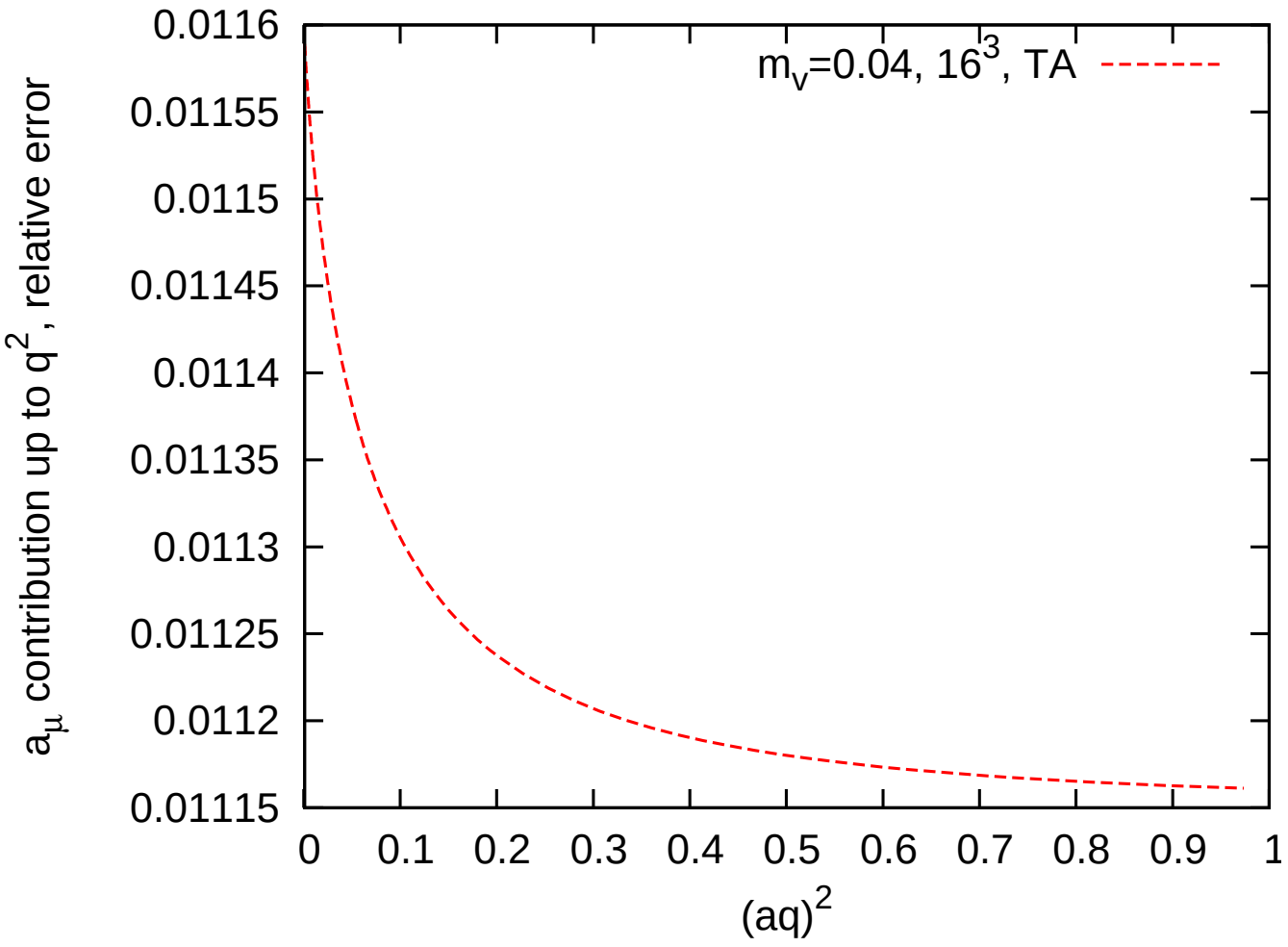
- Next: HVP and pion mass splitting at physical pion mass and second lattice spacing for continuum limit
- We will investigate g_A, multi-hadron states, and other quantities that may have large FV errors

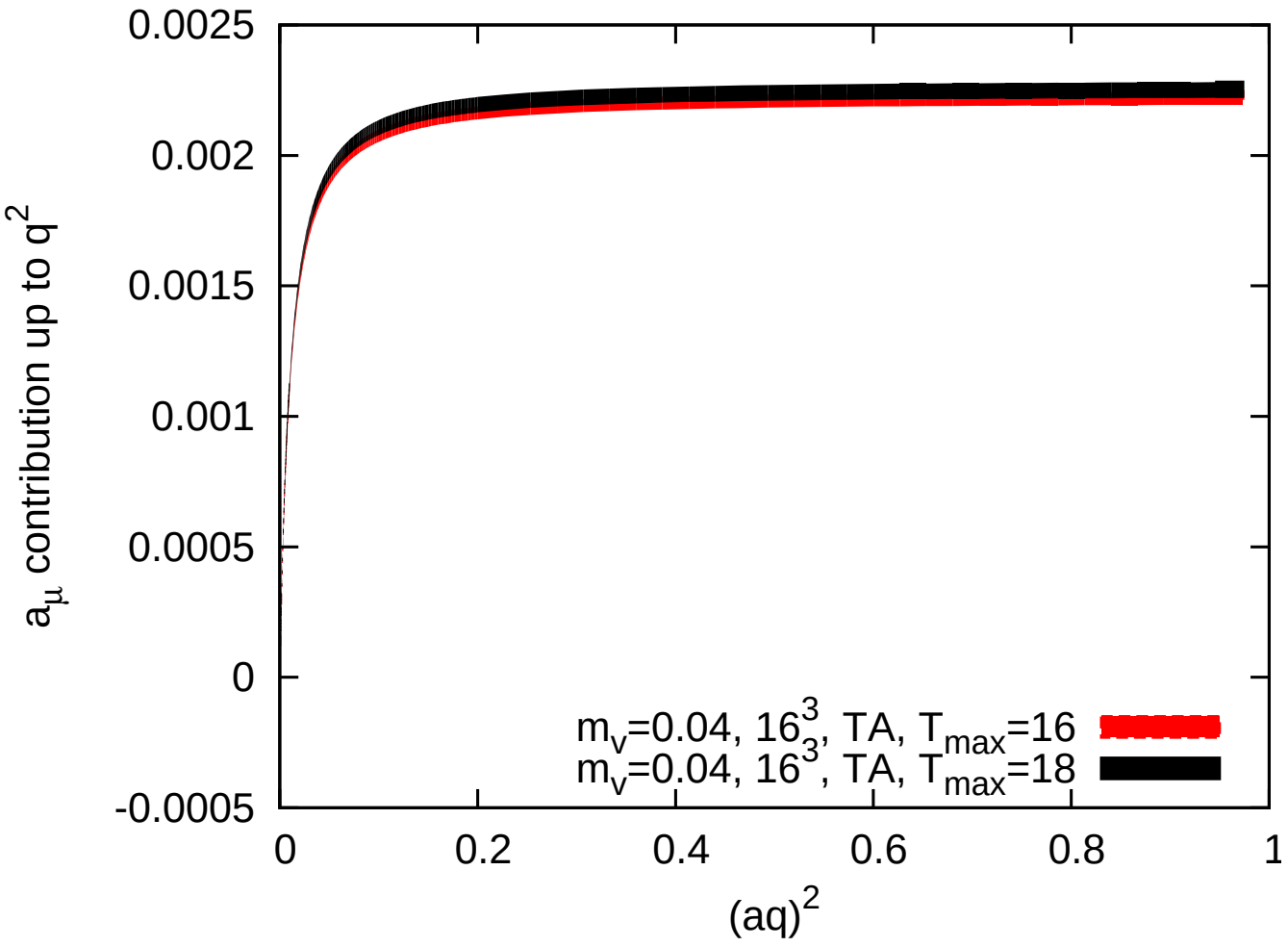
Thank you to our RBC/UKQCD colleagues

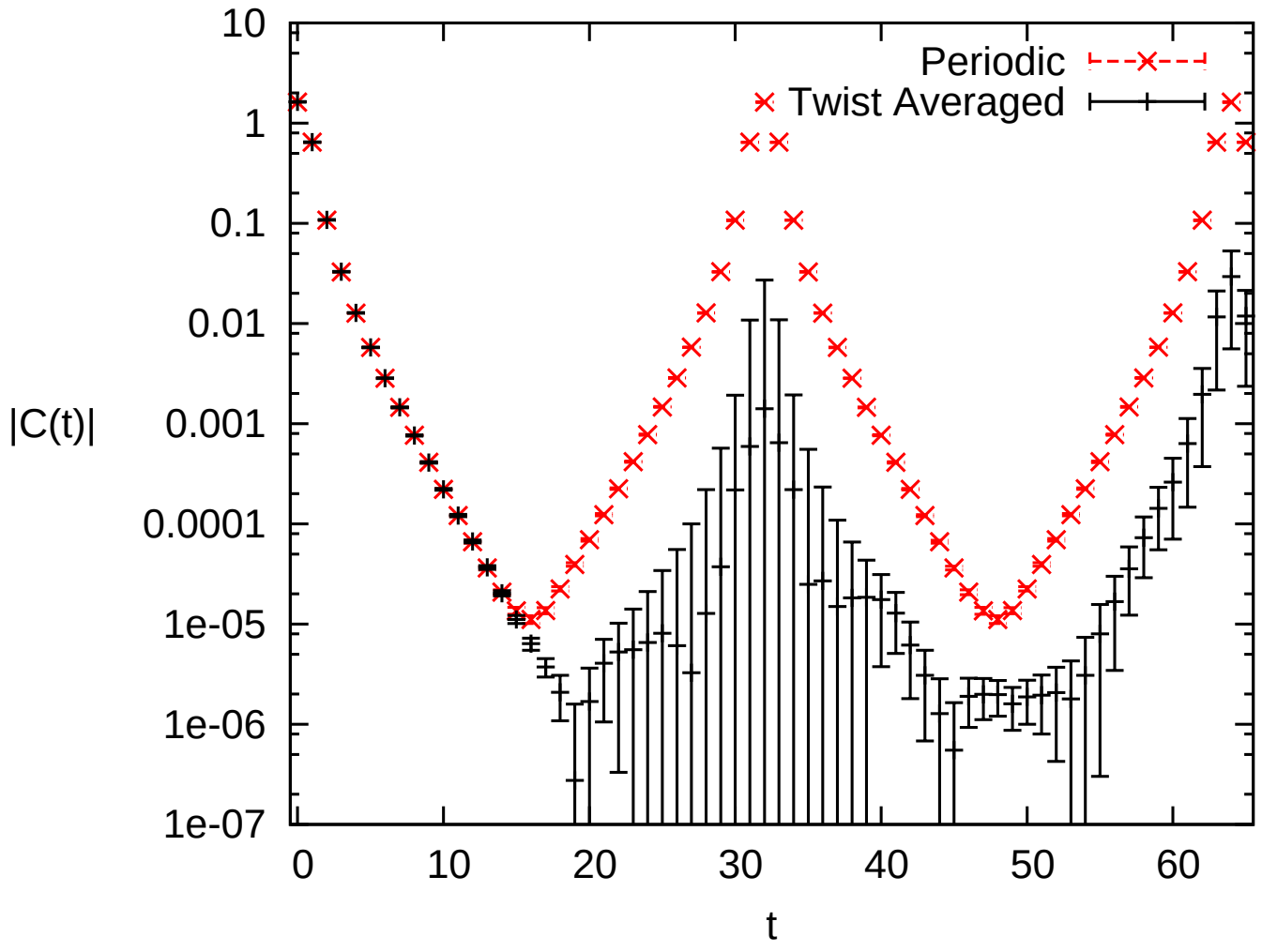
Backup slides

Detailed 16^3, strange quark plots


0.05
0
-0.05
-0.1
-0.15
-0.2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
a_μ contribution up to q^2, (T-S) / σ
$(aq)^2$
m_v=0.04, 16^3, TA


m_v=0.04, 16^3, TA
0.0116
0.01155
0.0115
0.01145
0.0114
0.01135
0.0113
0.01125
0.0112
0.01115
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
$(aq)^2$
a_μ contribution up to q^2, relative error


0.0025
0.002
0.0015
0.001
0.0005
0
-0.0005
0
0.2
0.4
0.6
0.8
1
a_μ contribution up to q^2
$(aq)^2$
m_V=0.04, 16^3, TA, T_{max}=16
m_V=0.04, 16^3, TA, T_{max}=18


Periodic
Twist Averaged
|C(t)|
t
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1
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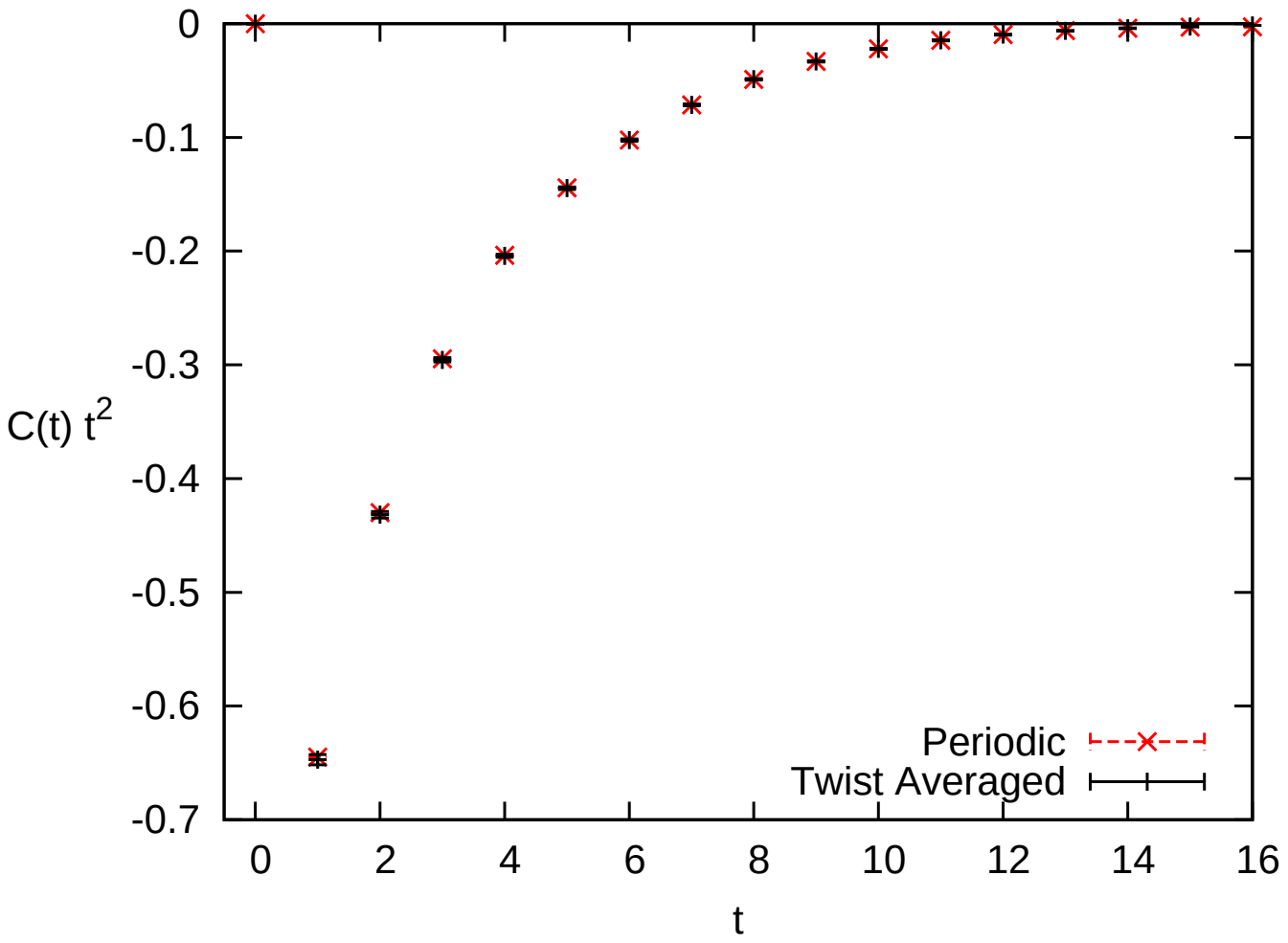
0
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C(t) t^2
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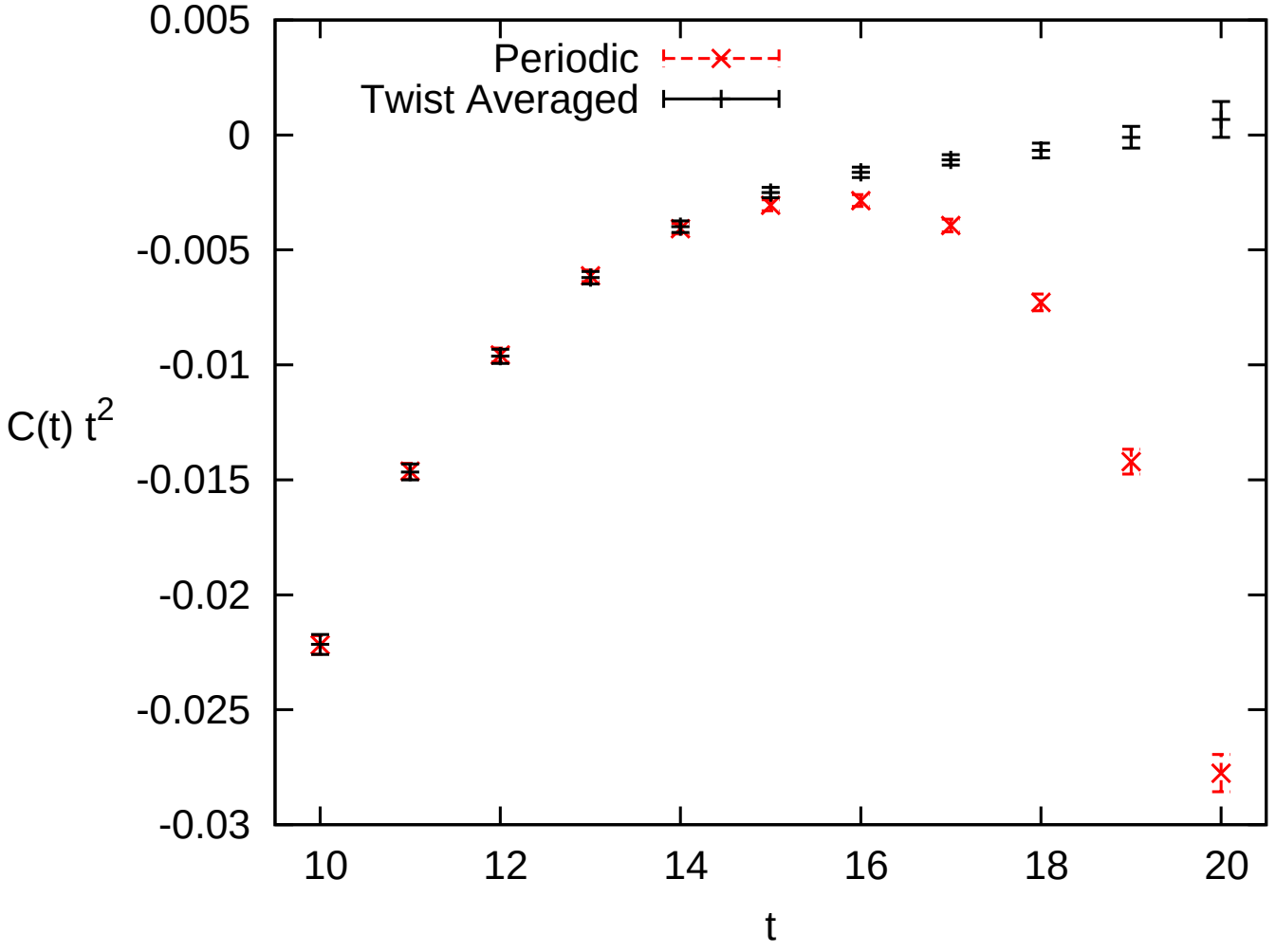
Periodic
Twist Averaged


Periodic
Twist Averaged
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-0.03
C(t) t^2
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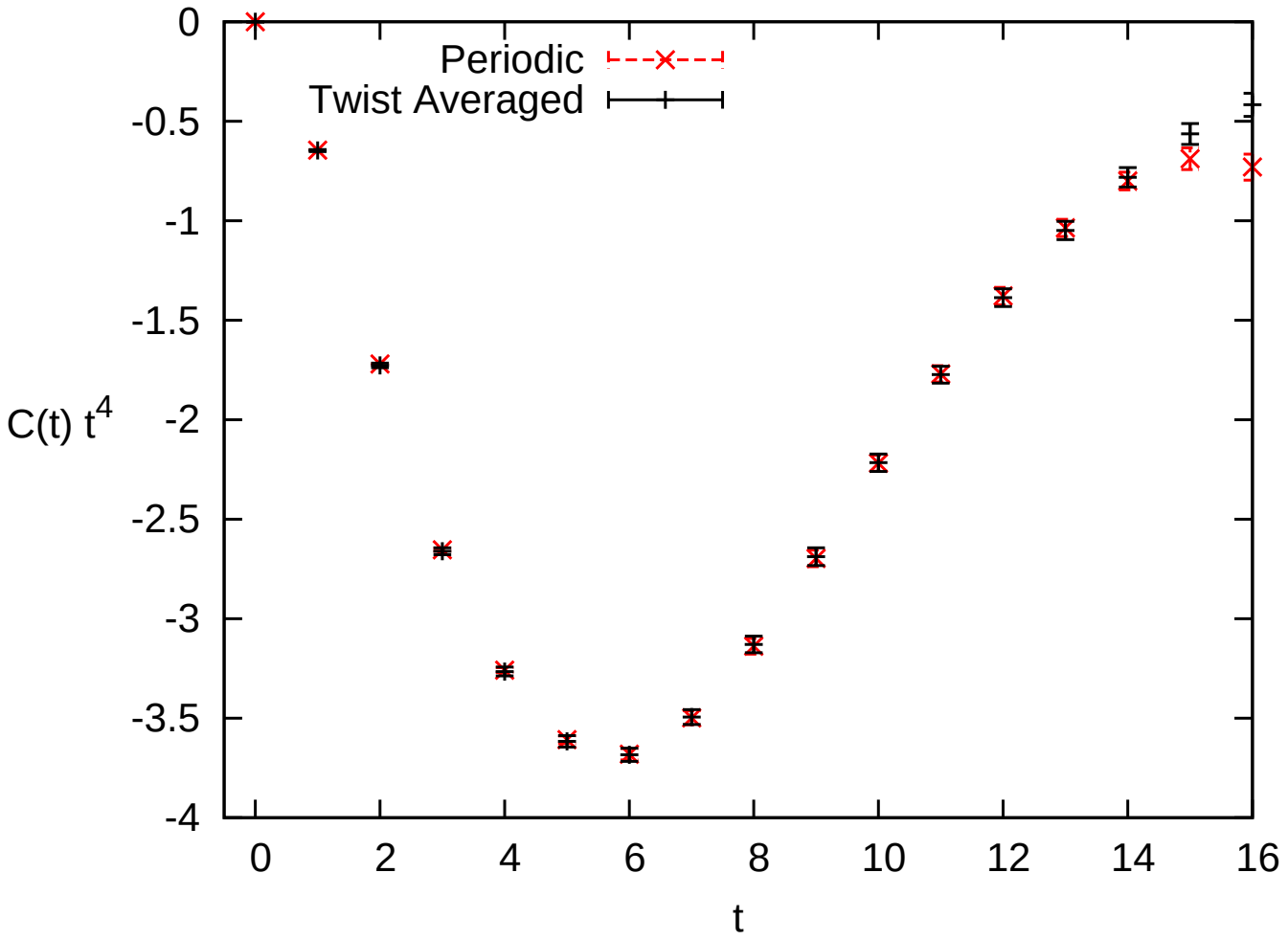
Periodic
Twist Averaged
C(t) t^4
t
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-1
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-4
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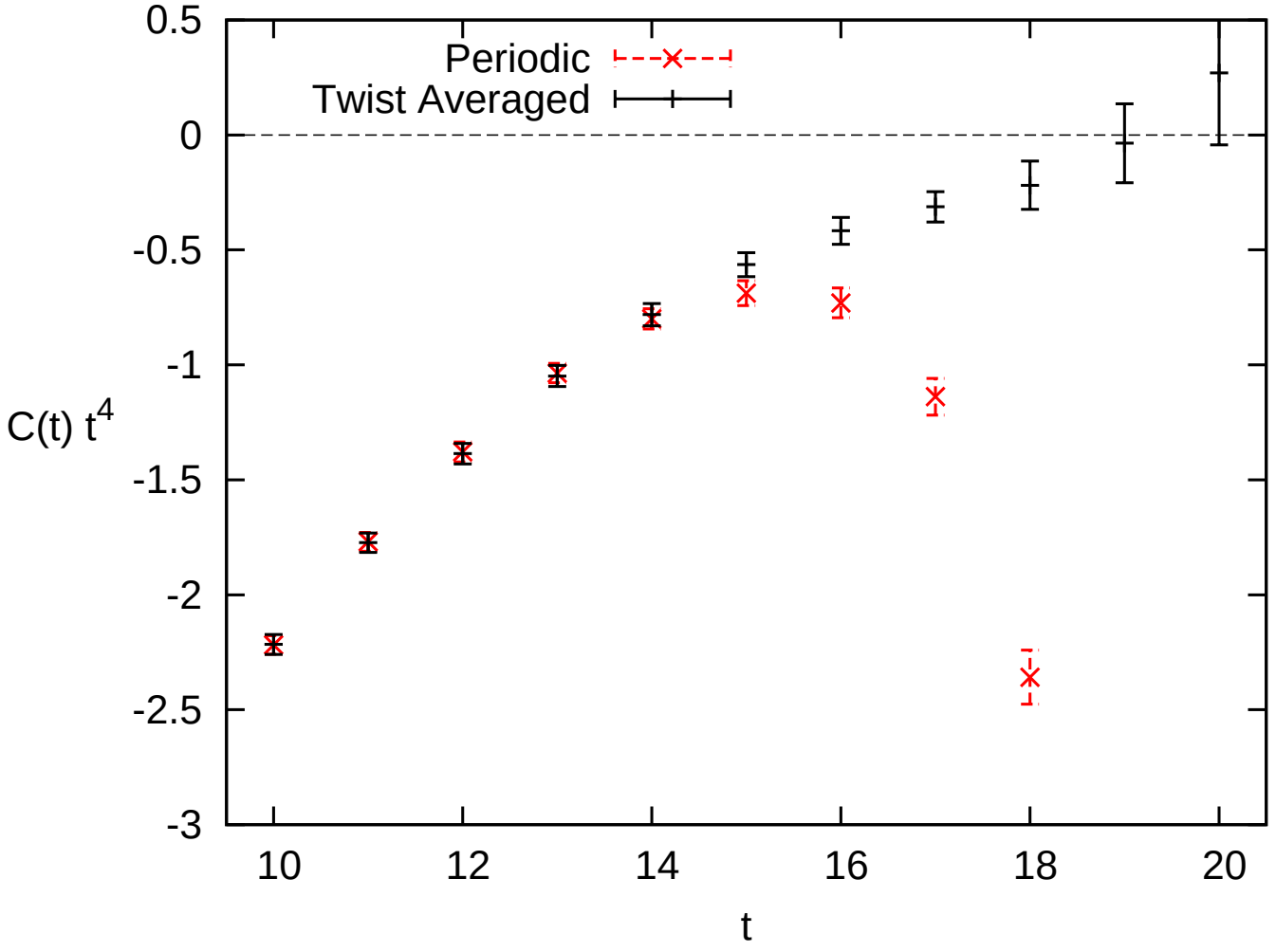
Periodic
Twist Averaged
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-3
C(t) t^4
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t