Neutron electric dipole moment with two flavors of domain wall fermions

Lattice 2005 (Dublin)

Tom Blum

(University of Connecticut and RIKEN BNL Research Center)

F. Berruto, K. Orginos(MIT), A. Soni(BNL)

(RBC Collaboration)

July 26, 2005

Outline

1. Introduction: physics and methodology*

2. Numerical results

3. Summary/Outlook

* Our calculation [Lattice 2004] is very similar to a recent quenched calculation [Aoki, Kikukawa, Kuramashi, and Shintani (2005)]. See also the talk by **E. Shintani** at this meeting.

Introduction

Consider adding a T- and P-odd (CP-odd) term to the QCD action

$$S_{QCD,\theta} = -\theta \int dt \int d^3x \, \frac{g^2}{32\pi^2} \mathrm{tr}\left[\epsilon_{\mu\nu\rho\sigma} G^{\mu\nu}(x) G^{\rho\sigma}(x)\right]$$

where $G^{\mu\nu}(x)$ is the gluon field strength and

$$\begin{aligned} \mathrm{Tr}\, G(x)\tilde{G}(x) &\sim \vec{E} \cdot \vec{B} \qquad (c.f., E^2 - B^2) \\ \tilde{G}(x)_{\mu\nu} &= \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} G^{\rho\sigma}(x) \end{aligned}$$

This "θ-term" gives rise to **permanent** electric dipole moments to the **quarks** as well as bound states like the **neutron**

The current **experimental bound** on d_N is
$|\vec{d}_N| < 6.3 \times 10^{-26}\, e$-cm [Harris, *et al.* (1999)]

New searches: ^{225}**Ra** (running at ANL) and **deuteron** (BNL proposal) to improve sensitivity by 2-3 orders of magnitude.

$+$ model calculations implies $\theta \lesssim 10^{-10}$, which is *unnaturally* small. This is often called the Strong CP problem.

Lattice regularization provides first-principles technique for calculation of d_N/θ.

The QCD Lagrangian for massless fermions

$$\mathcal{L}_{QCD,f} \;=\; \bar{\psi}\,(i\not{D})\,\psi$$

is invariant under chiral transformations of the quark fields

$$\begin{aligned} \psi &\rightarrow (1 + i\alpha\gamma_5/2)\psi \\ \bar{\psi} &\rightarrow \bar{\psi}(1 + i\alpha\gamma_5/2) \end{aligned}$$

But the measure of the path intergral is *not*,

$$\mathcal{D}\psi\mathcal{D}\bar{\psi} \;\rightarrow\; \mathcal{D}\psi\mathcal{D}\bar{\psi}\,\exp i\,\alpha \int d^4x\,\frac{g^2}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{Tr}G_{\mu\nu}G_{\rho\sigma}$$

which gives rise to the Adler-Bell-Jackiw anomaly
(*a.k.a* the axial anomaly, *c.f.* massive η' and $\pi^0 \rightarrow 2\gamma$).

Choosing $\alpha = -\theta$, the θ term can be **rotated away**, or canceled exactly in the action [But not for $N_f = 1$, see Creutz (2004)]

If all the quarks are **massive**, the chiral rotation generates another term in the action that can *not* be canceled by further field re-definitions

$$m\bar{\psi}\psi \;\; \rightarrow \;\; m\bar{\psi}\psi + i\theta m\bar{\psi}\gamma_5\psi$$

which is also P- and T- odd.

Thus the CP-violating term in the QCD Lagrangian can be transformed between the gauge and fermion sectors, but it can not be eliminated

The θ term can be written as a total divergence.

Still,

$$\int d^4x \frac{g^2}{32\pi^2} \mathrm{tr}\,\epsilon^{\mu\nu\rho\sigma} G_{\mu\nu} G_{\rho\sigma} \;=\; Q$$

where Q is the integral *topological charge*, $Q = 0, \pm 1, \pm 2, \ldots$

Thus the θ term can produce physical effects (like an electric dipole moment of the neutron)

Taking the chiral limit, $m \to 0$

Again, consider the QCD partition function for **massive** quarks which can be written

$$Z = \int \mathcal{D}A_\mu \ \mathrm{det}[\not{D}(m) + i\theta\overline{m}\gamma_5]^{N_f} \ e^{-S_G}.$$

and **if θ is small**,

$$\mathrm{det}\,[\not{D}(m) + i\theta m\gamma_5] = \mathrm{det}[\not{D}(m)]\ [1 + i\theta m\ \mathrm{tr}(\gamma_5 \not{D}(m)^{-1})\ ] + \mathcal{O}(\theta^2),$$

The spectral decomposition of $\not{D}(m)^{-1}$ and the index theorem lead to

$$\not{D}(m)^{-1} = \sum_\lambda \frac{|\lambda\rangle\langle\lambda|}{i\lambda + m}$$

$$\sum_{f=1}^{N_f} \mathrm{tr}\left[\gamma_5 \not{D}^{-1}(m)\right] = \frac{n_+ - n_-}{m} = \frac{Q}{m}$$

What happened? It appears that in the $m \to 0$ limit, the θ term does not vanish

Correct quark mass dependence is recovered from the usual CP-even part of the fermionic action,

$$\det \not{D}(m)^{N_f} \;=\; \Pi_i (i\lambda_i + m)^{N_f}$$

As $m \to 0$, $Q \neq 0$ configurations are **suppressed** since they support exact zero modes of $\not{D}$ with $\lambda_i = 0$.

In other words, the *distribution* of $Q \to \delta(Q)$, or $\langle Q^2 \rangle / V \to 0$, so the θ term effectively vanishes.

The quenched approximation of lattice QCD

Quenched approximation: set

$$\det[\not{D}(m)] = 1$$

(amounts to omitting quark vacuum polarization to all orders)

For small θ,

$$\det[\not{D}(m) + i\theta\overline{m}\gamma_5] = \det[\not{D}(m)]\,[1 + i\theta\overline{m}\ \mathrm{tr}(\gamma_5\not{D}(m)^{-1})\,] + \mathcal{O}(\theta^2),$$

So, even in quenched case there is CP-violating physics [Aoki, Gocksch, Manohar, and Sharpe (1990)]. But **mass dependence is completely wrong**. Many observables, possibly d_N, have pathological chiral limit (*c.f.*, d_N in ILM [Faccioli, Guadagnoli, Simula (2004)])

Computational Methodology

Compute the matrix elements of the *electromagnetic current* between nucleon states in the $\theta \neq 0$ vacuum

$$\begin{aligned}\langle p', s'|J^\mu|p, s\rangle_\theta &= \bar{u}_{s'}(p')\Gamma^\mu(q^2)u_s(\vec{p})\\ \Gamma^\mu(q^2) &= \gamma^\mu F_1(q^2) + i\,\sigma^{\mu\nu}q_\nu \frac{F_2(q^2)}{2m}\\ &\quad + \left(\gamma^\mu\gamma^5 q^2 - 2m\gamma^5 q^\mu\right) F_A(q^2) + \sigma^{\mu\nu}q_\nu\gamma^5 \frac{F_3(q^2)}{2m}\end{aligned}$$

$$\begin{aligned}J^\mu &= \frac{2}{3}\bar{u}\gamma^\mu u - \frac{1}{3}\bar{d}\gamma^\mu d = \frac{1}{2}J_V^\mu + \frac{1}{6}J_S^\mu\\ J_V^\mu &= \bar{u}\gamma^\mu u - \bar{d}\gamma^\mu d\\ J_S^\mu &= \bar{u}\gamma^\mu u + \bar{d}\gamma^\mu d.\end{aligned}$$

$q^2 < 0$, momentum transfered by the external photon (space-like)

The most general matrix element consistent with **Lorentz, gauge, CPT** symmetries of QCD. The insertion of J^μ probes the electromagnetic structure of the nucleon. For $q^2 \to 0$

- $F_1(0)$: electric charge in units of e (+1 proton, 0 neutron)
- $F_2(0)/2m$: magnetic dipole moment in units of e
- F_A: anapole moment
- $F_3(0)/2m$: electric dipole moment in units of e

The last two vanish if $\theta = 0$

Calculating dipole moments on the lattice

Lattice calculations are done with *correlation functions* in Euclidean space-time,

and rely on the LSZ reduction formula to project out the desired matrix element by using exponential dominance of ground state

$$
\begin{aligned}
G(t,t') &= \langle \chi_N(t',\vec{p}')\, J^\mu(t,q)\, \chi_N^\dagger(0,\vec{p}) \rangle \\
&= \sum_{s,s'} \langle 0|\chi_N|p',s'\rangle \langle p',s'|J^\mu|p,s\rangle \langle p,s|\chi_N^\dagger|0\rangle \frac{1}{2E\,2E'} e^{-(t'-t)E'} e^{-tE} \\
&\quad + \ldots \\
&= G^\mu(q) * f(t,t',E,E') + \ldots
\end{aligned}
$$

With suitable choices of *projectors*, form factors can be determined from the correlation functions, $e.g.$ for $\theta = 0$,

$$
\begin{aligned}
\mathcal{P}^{xy} &= -\frac{i}{4}\frac{1+\gamma^4}{2}\gamma^x\gamma^y \\
\mathcal{P}^{4} &= \frac{1}{4}\frac{1+\gamma^4}{2}\gamma^4 \\
&= \frac{1}{4}\frac{1+\gamma^4}{2} \\
\mathrm{tr}\mathcal{P}^{xy}\, G^{x,y}(q^2) &= \pm p_{y,x}\, m(F_1(q^2) + F_2(q^2)) \\
\mathrm{tr}\mathcal{P}^{4}\, G^{4}(q^2) &= m\,(E+m)\left(F_1(q^2) + \frac{q^2}{(2m)^2}F_2(q^2)\right)
\end{aligned}
$$

Linear combinations of F_1 and F_2 in ()'s are **magnetic and electric form factors**, $G_M(q^2)$ and $G_E(q^2)$, respectively.

To get the desired moment **take ratios** of three-point functions (Z, renormalization, kinematical factors all drop out), *e.g.*,

$$\begin{aligned}\lim_{t'\gg t\gg 0}\frac{1}{p_y}\frac{\mathrm{tr}\mathcal{P}^{xy}G^x_{P,N}(t,t',E,\vec{p})}{\mathrm{Tr}\mathcal{P}^4G^4_P(t,t',E,\vec{p})} &= \frac{1}{p_y}\frac{\mathrm{tr}\mathcal{P}^{xy}G^x_{P,N}(q^2)}{\mathrm{tr}\mathcal{P}^4G^4_P(q^2)} \\ &= \frac{1}{E+m}\frac{F_1(q^2)+F_2(q^2)}{G_E^{(P)}(q^2)} \\ \lim_{q\to 0} &= \frac{1}{2m}\begin{cases}1+a_{\mu,P}\\ a_{\mu,N}\end{cases}\end{aligned}$$

yields the magnetic dipole moments

$F_1(0)=1$, 0 for the proton, neutron

CP violating vacuum, $\theta \neq 0$

The **physical** neutron in the CP-broken vacuum is a **mixture** of the $\theta = 0$ vacuum (opposite parity) eigenstates $|N\rangle$ and $|N^*\rangle$.

$$
\begin{aligned}
|N^\theta\rangle &= |N\rangle + i\alpha'|N^*\rangle \\
\alpha' &\propto \theta
\end{aligned}
$$

This gives rise to mixing of electric and magnetic dipole moment terms in projected correlation functions.

[Pospelov and Ritz (1999), Aoki, Kikukawa, Kuramashi, and Shintani (2004)]

The **electric dipole moment** is obtained from, *e.g.*

$$
\begin{aligned}
\mathrm{tr}\mathcal{P}^{xy}\, G^z(q^2) &= \alpha m(E-m)F_1 + \alpha(m(E-m)+\frac{p_z^2}{2})F_2 + \frac{p_z^2}{2}F_3 + \mathcal{O}(\theta^2) \\
\mathrm{tr}\mathcal{P}^{xy}\, G^t(q^2) &= ip_z\left(\alpha m F_1(q^2) + \alpha\frac{E+3m}{2}F_2(q^2) + \frac{E+m}{2}F_3(q^2)\right) \\
&\quad +\mathcal{O}(\theta^2).
\end{aligned}
$$

The terms proportional to α must be subtracted

$$
\begin{aligned}
\left\{\frac{1}{ip_z}\frac{\mathrm{tr}\mathcal{P}^{xy}G_N^t(t,t',E,\vec{p})}{\mathrm{tr}\mathcal{P}^t G_P^t(t,t',E,\vec{p})} - \frac{\alpha m F_1(q^2) + \alpha\frac{E+3m}{2}F_2(q^2)}{m(E+m)G_E^{(P)}(q^2)}\right\} &= \frac{F_3(q^2)}{2mG_E^{(P)}(q^2)} \\
\lim_{q^2\to 0}\{\cdots\} &= \frac{F_3(0)}{2m} = d_N
\end{aligned}
$$

Mixing angle α is calculated from the
ratio of two-point functions
[Aoki, Kikukawa, Kuramashi, and Shintani (2004)]

$$\langle \chi_{N^\theta}(t)\chi^\dagger_{N^\theta}(0)\rangle_\theta \;=\; \frac{Z_{N^\theta}(1+\gamma^4+\exp i2\alpha\gamma^5)}{2}\exp -m_{N^\theta}t + \ldots$$

To lowest order in α (θ) we have

$$\mathrm{tr}\frac{1+\gamma^4}{2}\gamma_5 \;\; \langle \chi_{N^\theta}(t)\chi^\dagger_{N^\theta}(0)\rangle_\theta \;\approx\; i\,Z_N\,\alpha\,e^{-m_N\,t}$$
$$\mathrm{tr}\frac{1+\gamma^4}{2} \;\; \langle \chi_{N^\theta}(t)\chi^\dagger_{N^\theta}(0)\rangle_\theta \;\approx\; Z_N\,e^{-m_N\,t}$$

$$m_{N^\theta} \;=\; m_N + \mathcal{O}(\theta^2)$$
$$Z_{N^\theta} \;=\; Z_N + \mathcal{O}(\theta^2)$$

Computing with $\theta \neq 0$

$$\langle \mathcal{O} \rangle_\theta \;=\; \frac{1}{Z(\theta)} \int \mathcal{D}\mathcal{A}_\mu \mathcal{D}\bar{\psi}\mathcal{D}\psi \mathcal{O}\, e^{-S(\mathcal{A}_\mu) - i\theta \int d^4x \, \frac{g^2}{32\pi^2} \mathrm{tr}[G(x)\tilde{G}(x)]}$$

Assuming $\theta \ll 1$

$$\approx \; \frac{1}{Z(0)} \int \mathcal{D}\mathcal{A}_\mu \mathcal{D}\bar{\psi}\mathcal{D}\psi (1 - i\theta Q) \mathcal{O}\, e^{-S(\mathcal{A}_\mu)}$$

$$= \; \langle \mathcal{O} \rangle - i\theta \langle Q \mathcal{O} \rangle$$

CP odd piece: simple weighted average in CP even vacuum

$$\langle Q \mathcal{O} \rangle \;=\; \sum_\nu P(Q_\nu)\; Q_\nu \;\langle \mathcal{O} \rangle_\nu,$$

Can also weight with the *pseudo-scalar density*

[Guadagnoli, Lubicz, Martinelli, and Simula (2002)]

For chirally symmetric lattice fermions that have an index, this is equivalent to weighting with Q. If chiral symmetry is broken, then the two methods will agree in the limit $a \to 0$.

Relation between d_N and topology of the vacuum

- $d_N \to 0$ as $m_\pi^2 \to 0$ since $\Pi_i(\lambda_i + m) \to 0$, $\lambda_i = 0$ for $Q \neq 0$

- χPT gives $d_N \sim m_\pi^2 \log m_\pi^2$, $\langle Q^2 \rangle / V \sim m_\pi^2$

- $\langle Q^2 \rangle / V =$ constant implies that d_N *does not vanish* in the quenched theory ($N_f = 0$) (pathological?)

- mixing angle α must vanish as $m_\pi^2 \to 0$;
  $\alpha \to 0$ as $\langle Q^2 \rangle / V \to 0$

- In large N, $\langle \mathcal{O} Q \rangle = \langle Q^2 \rangle \frac{\partial \langle \mathcal{O} \rangle}{\partial Q} \Big|_{\nu=0} = \langle Q^2 \rangle \langle \mathcal{O} \rangle_{\nu=1}$ [Diakonov, *et al.* (1996); Faccioli, *et al.* (2004)]

Numerical Results

- DWF+DBW2, $N_f = 2$, $m_{\text{sea}} = m_{\text{val}} = 0.04$ [RBC Collaboration (2004)].

- $m_{\text{sea}} = 0.02$ and 0.03 in progress

- $a^{-1} \approx 1.7$ GeV.

- quenched DWF+DBW2, $m_{\text{val}} = 0.05$ valence DWF [RBC Collaboration (2002)]

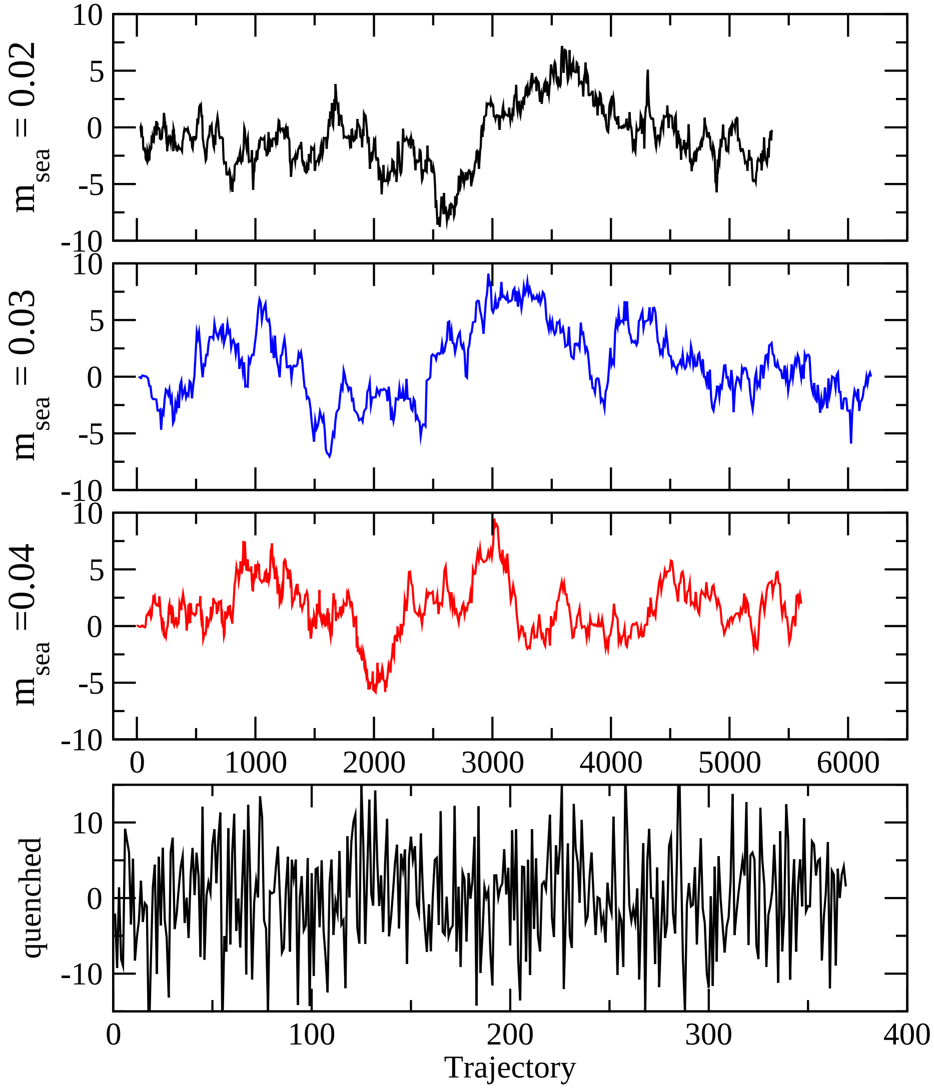
- Non-zero momenta for one of the nucleons, $\vec{p} = (\pm 1, 0, 0)$, $(\pm 1, \pm 1, 0)$, and $(\pm 1, \pm 1, \pm 1)$ (and permutations) since form factors multiplied by q^ν
($\partial/\partial(q^2)|_0$ not accessible on a finite lattice [Wilcox (2002)])

Topological charge "history" (distribution):

$N_f = 2$ flavor: small step hybrid monte-carlo, Q sampled **slowly**, **long-time** correlations

Quenched: big change heat bath monte-carlo, Q sampled **efficiently**, $\sim$ **no** correlations

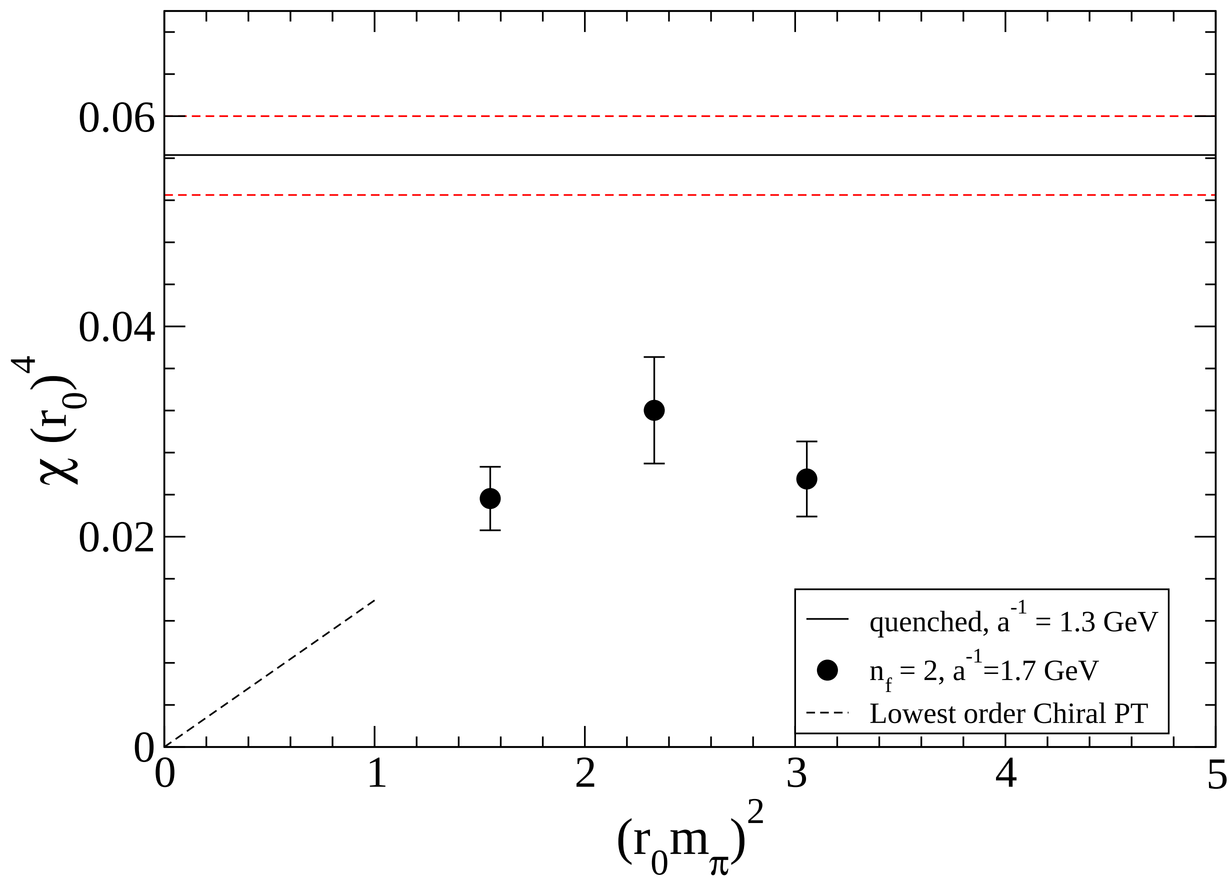
$\mathcal{O}(a^2)$ improved Q was computed by integrating the topological charge density after APE smearing the gauge fields.



Topological charge susceptibility χ:

$$\chi = \frac{\langle Q^2 \rangle}{V} = f^2 m_\pi^2 / 8$$

Statistical errors may be under-estimated (blocks of 50 trajecs)

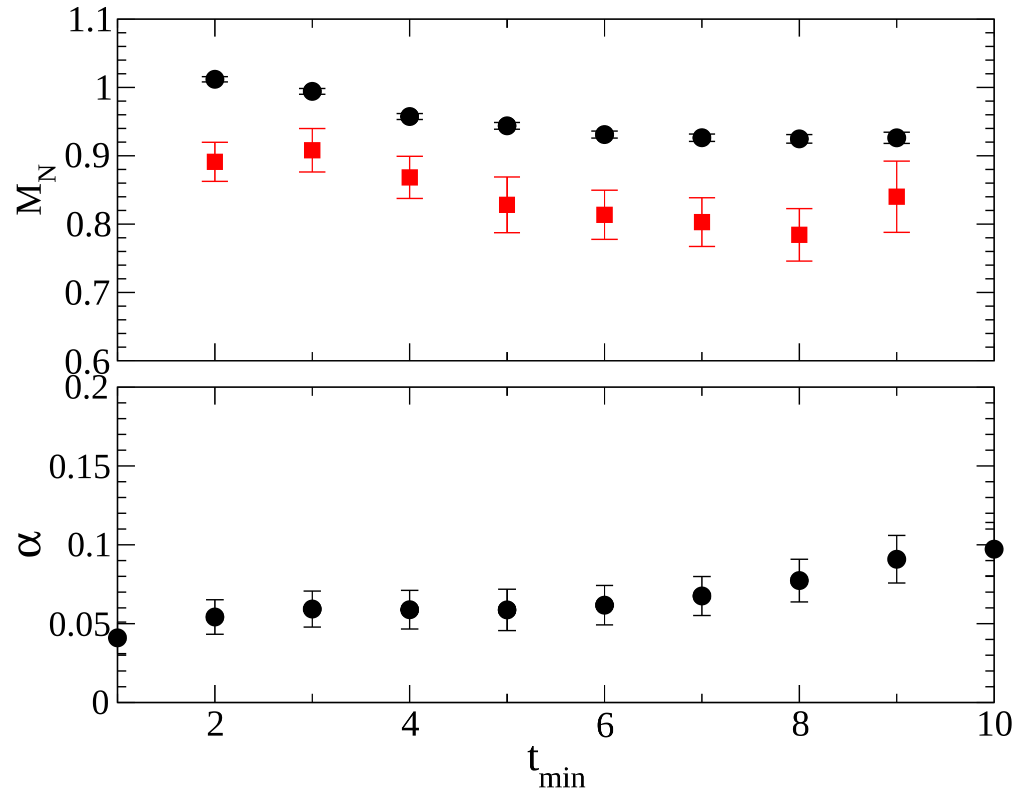


The mixing coefficient α

To lowest order in θ, CP even and odd parts of two point function have the same mass, m_N, and amplitude.

$$G(t) = A\, e^{-m_N\, t} + \cdots$$
$$G_\theta(t) = A\, \alpha\, e^{-m_N\, t} + \cdots$$

Systematic **difference** in nucleon mass determination makes extraction of α difficult: **fake** plateau

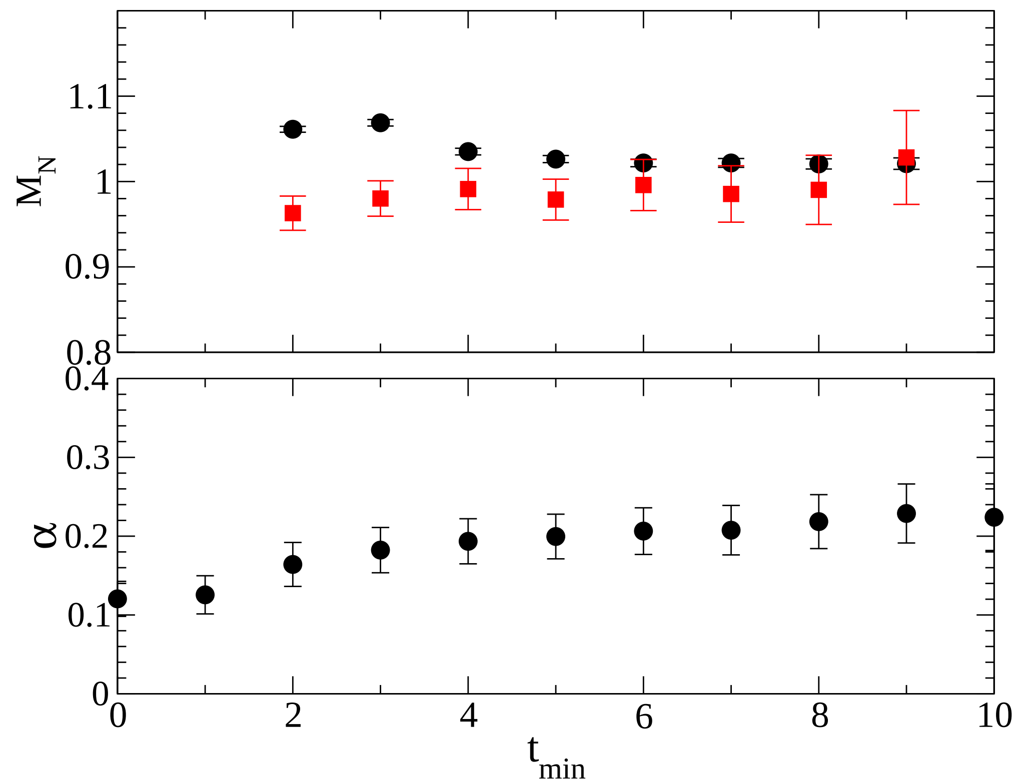


mixing coefficient α, quenched

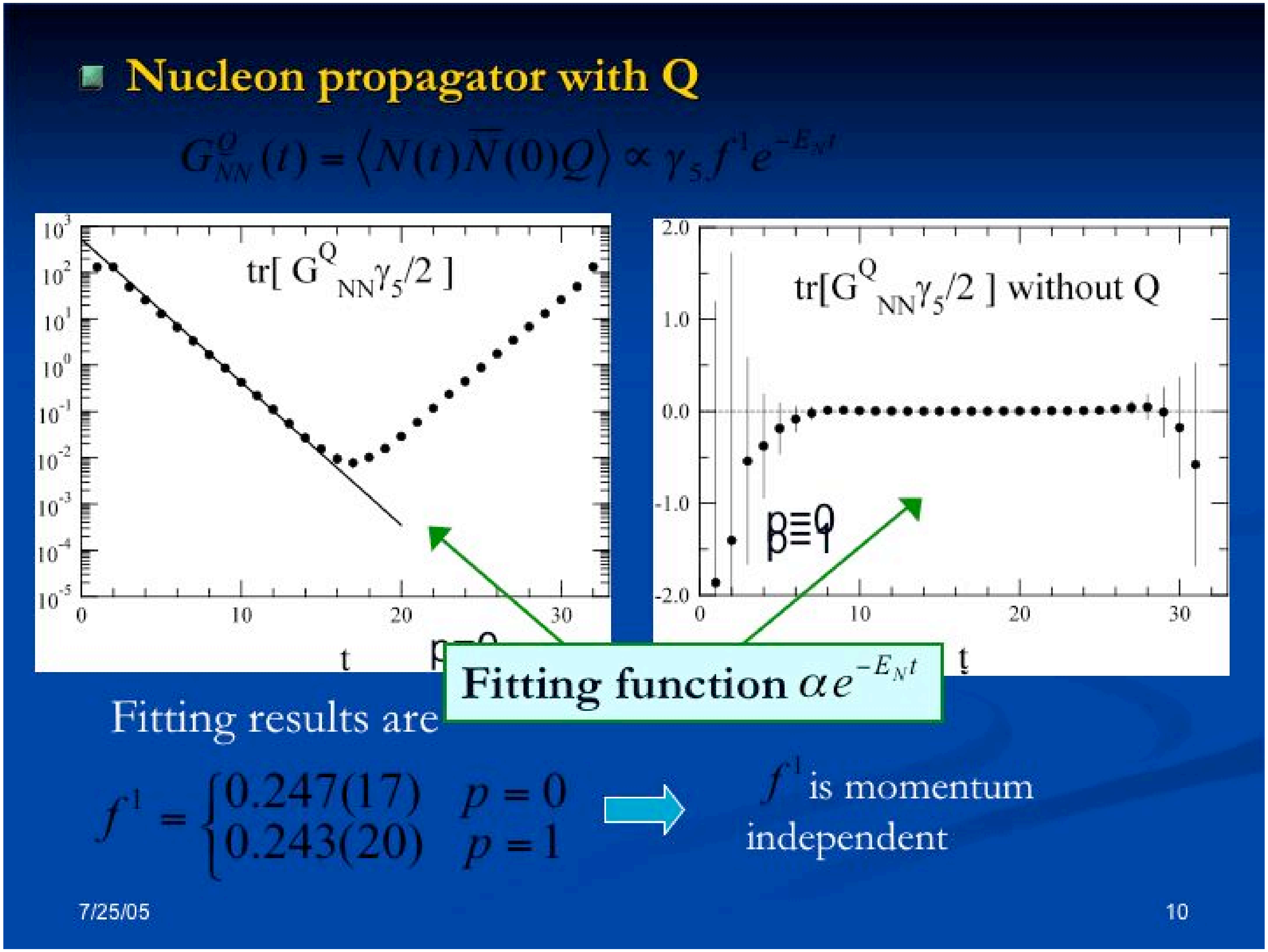
Things look more sensible on the **quenched** lattice: better sampling of topological charge.

Plateau is (almost) trustworthy.

α = 0.21(3) is rather large, *c.f.* topological charge susceptibility



Eigo Shintani's talk: reweighting with Q is non-trivial, but works!



mixing coefficient α, $N_f = 2$ again

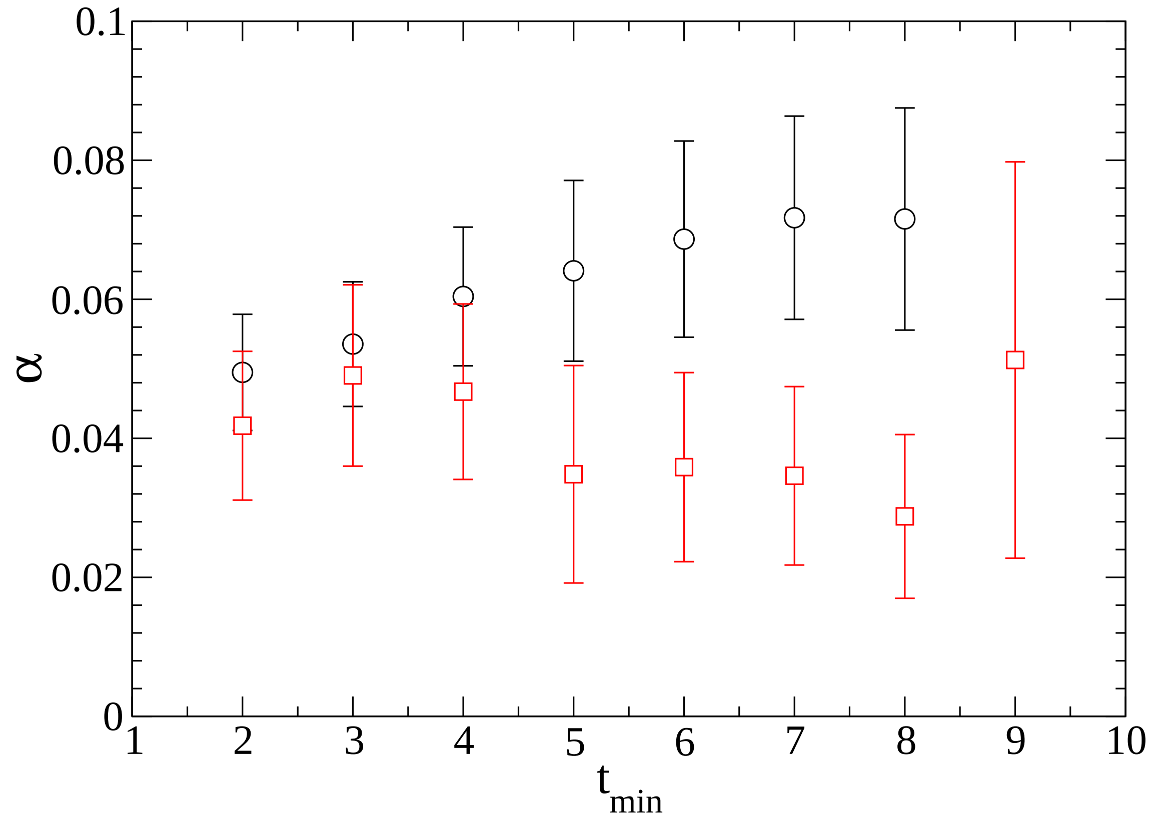
Extract α **from fit** $G_\theta(t) = A\,\alpha\,e^{-m_N\,t}$.

$$\alpha \;=\; 0.035(13)$$

Can also **fix** m_N to its **correct** CP even value

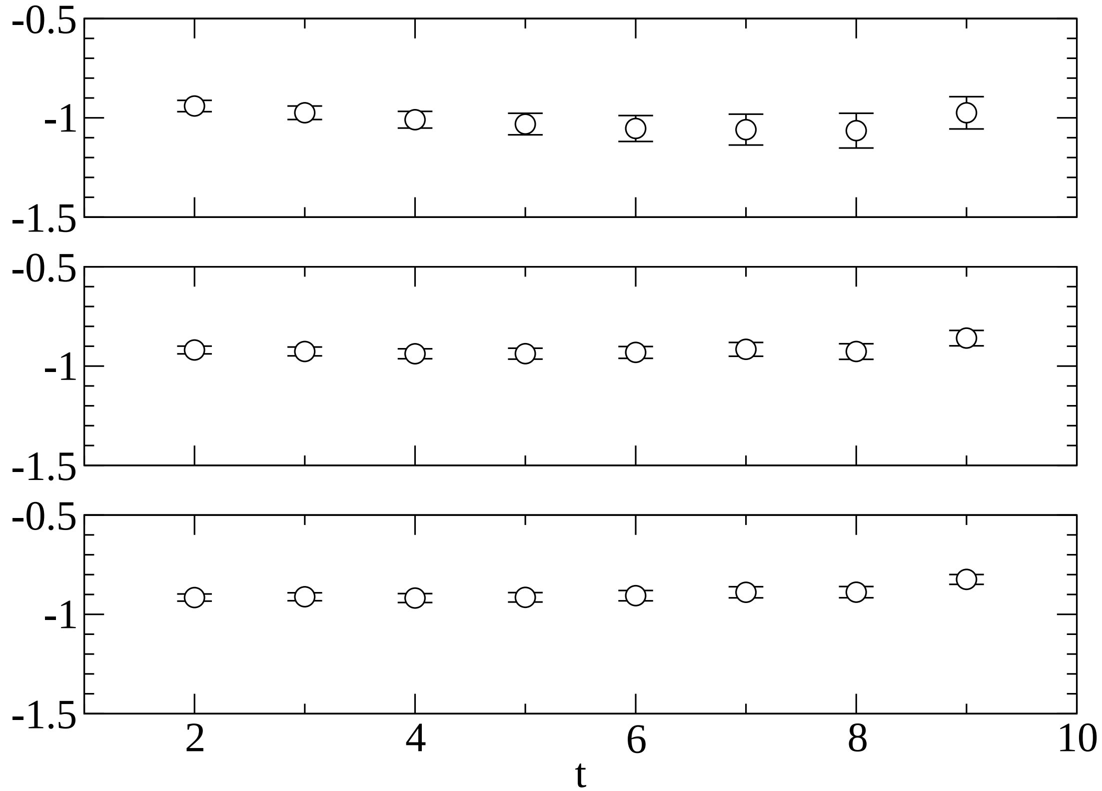
$$\alpha \;=\; 0.072(15)$$

Imprecise, but much **smaller** than quenched value (*c.f.*, $\langle Q^2/V\rangle$)



Three-point correlation function ratios

- Neutron **magnetic form factor** ratios
- Nucleon sources at $t = 0$ and 10
- Excited state contamination appears small
- lowest q^2 on the bottom

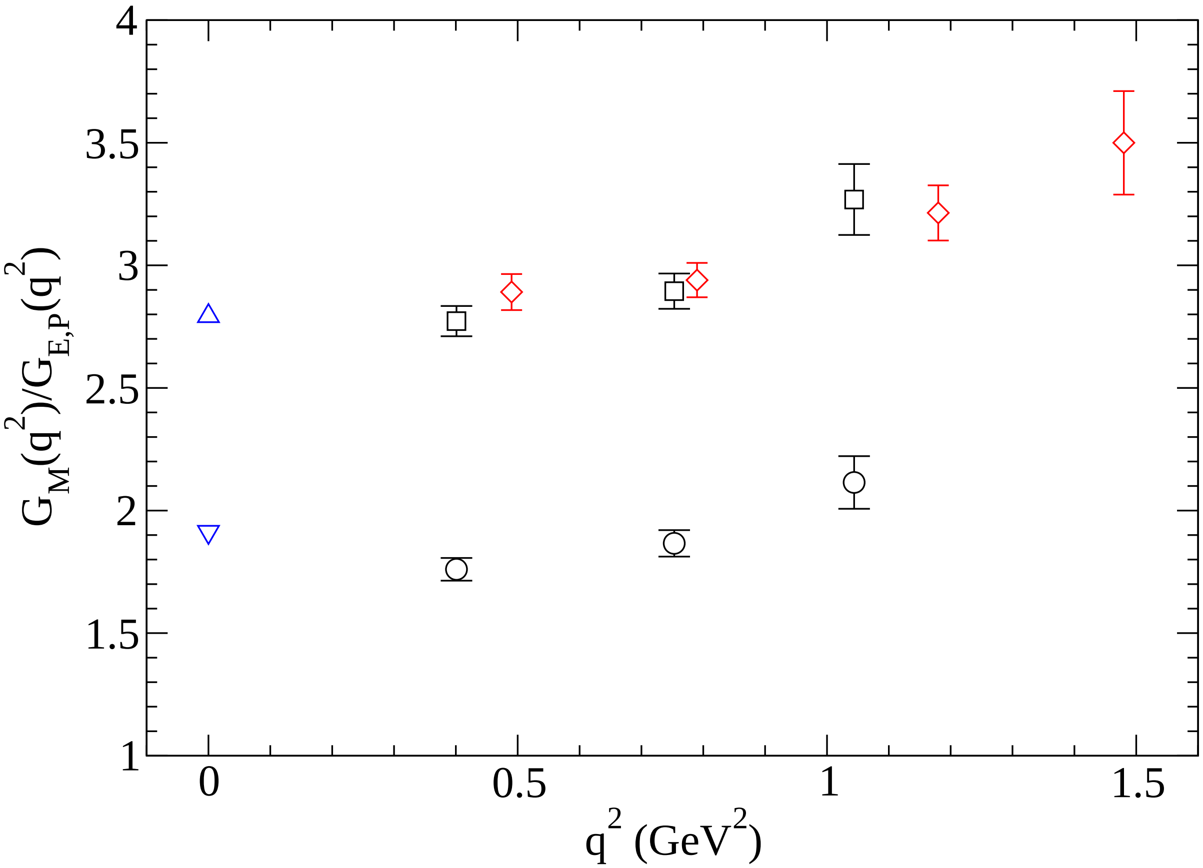


Ratio of form factors $G_M(q^2)/G_E^{(P)}(q^2)$

q^2 dependence mild

Reasonable agreement with experiment (diamonds) [Jones, *et al.* (2000), JLab]

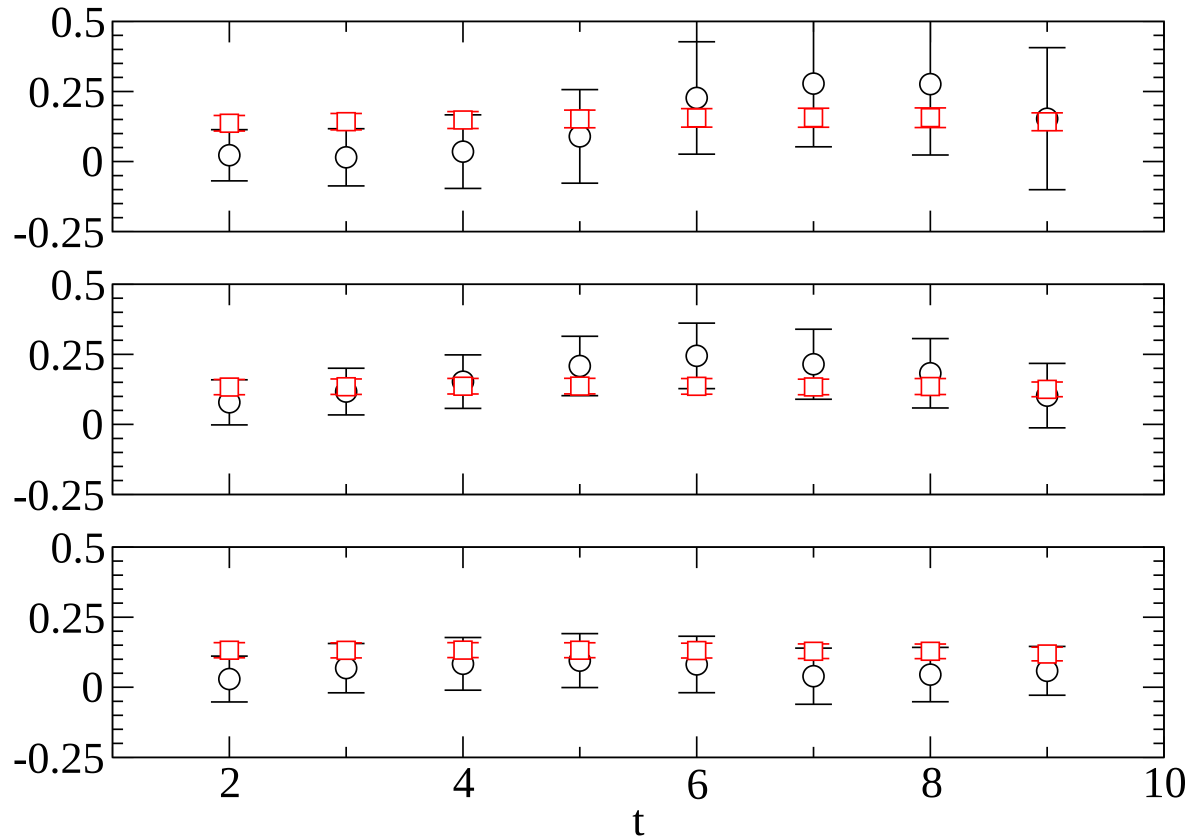
Anomalous μ's are **equal and opposite** well within errors, implies iso-scalar contribution ~ 0; **disconnected** diagrams not computed, so puzzling



(Lattice error estimates are statistical uncertainties only)

Subtracted $F_3(q^2)$ ratios

- Neutron **electric dipole form factor** ratios
- F_1 and F_2 terms subtracted
- Subtraction term (squares) is relatively well resolved
- error dominated by 3-point function, ~ 0



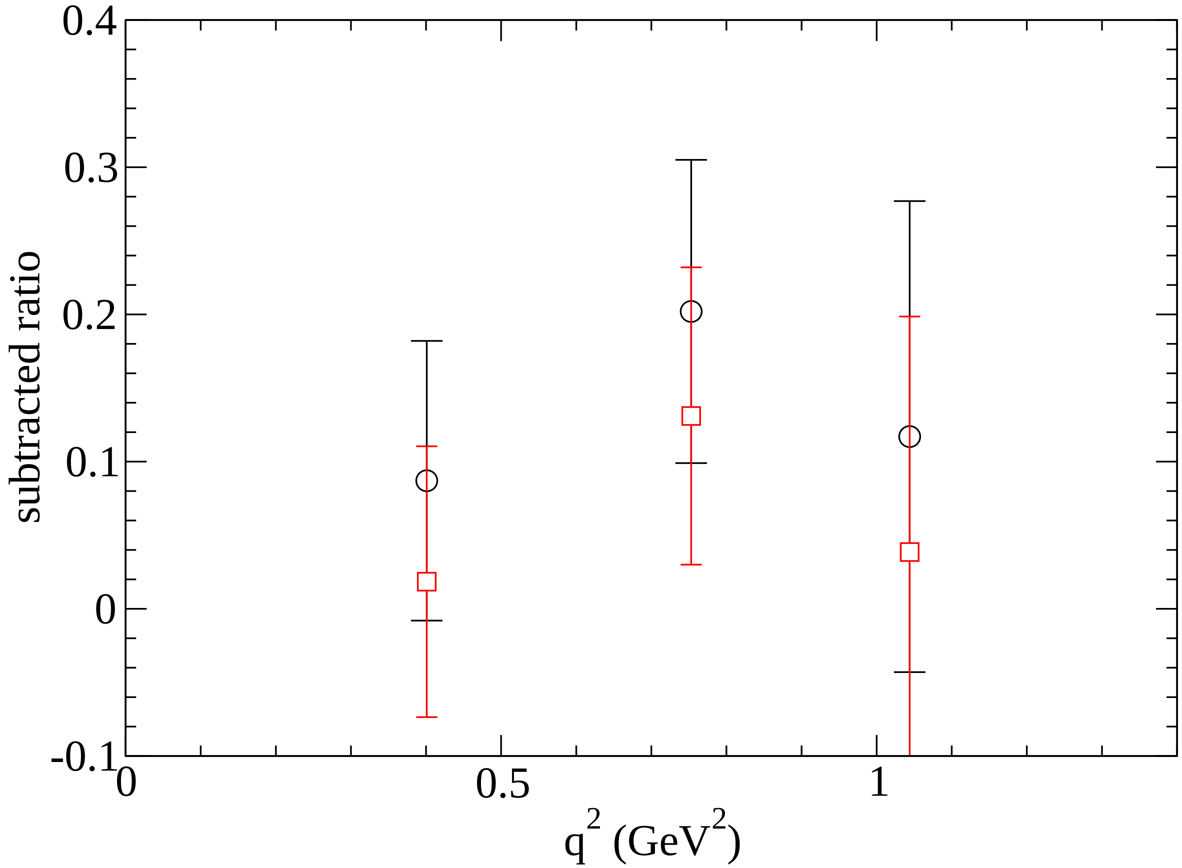
Ratio of form factors $F_3(q^2)/(2mG_E^{(P)}(q^2))$

$$d_N^{\text{lat}} = \frac{F_3(0)}{2m} \approx \frac{F_3(0.401\,\text{GeV}^2)}{2m} = +0.087(95).$$

Our conventions have lead to a **positive** central value of d_N/θ. Could change as calculation improves.

In physical units,

$$d_N \approx 0.010(11)\,\theta\, e\ \text{fm}.$$



(Error estimates are statistical uncertainties only.)

Summary/Outlook

Inadequate topological charge distribution limits the accuracy of the $N_f = 2$ flavor calculation (algorithmic problem).

Quenched calculation avoids this problem, but χ is unphysically large and has the wrong quark mass dependence, so quenched d_N will have large systematic error.

Our central value is $\sim 2\times$ **leading χPT** result [Crewther, Di Veccio, Veneziano, Witten (1979)], $\sim 5 - 10\times$ **sum rules** value [Pospelov and Ritz (1999)], $\sim -0.4\times$ **quenched** value [Aoki, Kikukawa, Kuramashi, and Shintani (2005)]

Future: In progress 2+1 flavor DWF calculation (RBC+UKQCD) may be promising if long HMC evolutions obtained [Talk by Yamaguchi, this meeting]. Need to carefully study the mass dependence, extrapolate to the physical pion (light quark) mass

Acknowledgements

The computations described here were done on the RIKEN BNL Research Center QCDSP supercomputer.

We thank our colleagues in the RBC collaboration, in particular N. Christ, M. Creutz, and S. Aoki for useful discussions.

The work of FB and AS was supported in part by US DOE grant # DE-AC02-98CH10886. KO was supported in part by DOE grant #DFFC02-94ER40818. TB was supported by the RIKEN BNL Research center.