Neutron electric dipole moment
with two flavors of domain wall fermions

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

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

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

$$\text{Tr} \, G(x) \tilde{G}(x) \sim \vec{E} \cdot \vec{B} \quad (c.f., E^2 - B^2)$$

$$\tilde{G}(x)_{\mu\nu} = \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} G^{\rho\sigma}(x)$$

This “$\theta$-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 $|\vec{d}_N| < 6.3 \times 10^{-26} \text{ e-cm} \ [\text{Harris, et al. (1999)}]$

New searches: $^{225}\text{Ra}$ (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 $d_N/\theta$. 
The QCD Lagrangian for massless fermions

\[ \mathcal{L}_{QCD,f} = \bar{\psi} (i\slashed{D}) \psi \]

is invariant under chiral transformations of the quark fields

\[
\begin{align*}
\psi & \rightarrow (1 + i\alpha \gamma_5/2)\psi \\
\bar{\psi} & \rightarrow \bar{\psi}(1 + i\alpha \gamma_5/2)
\end{align*}
\]

But the measure of the path integral is not,

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

which gives rise to the Adler-Bell-Jackiw anomaly (a.k.a the axial anomaly, c.f. massive \( \eta' \) and \( \pi^0 \rightarrow 2\gamma \)).
Choosing $\alpha = -\theta$, the $\theta$ 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 redefinitions

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

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 $\theta$ term can be written as a total divergence.

Still,

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

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

Thus the $\theta$ 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

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

and if $\theta$ is small,

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

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

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

$$\sum_{f=1}^{N_f} \text{tr} [\gamma_5 \not{D}^{-1}(m)] = \frac{n_+ - n_-}{m} = \frac{Q}{m}.$$
What happened? It appears that in the $m \to 0$ limit, the $\theta$ term does not vanish.

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

$$\det \mathcal{D}(m)^{N_f} = \prod_i (i \lambda_i + m)^{N_f}$$

As $m \to 0$, $Q \neq 0$ configurations are **suppressed** since they support exact zero modes of $\mathcal{D}$ with $\lambda_i = 0$.

In other words, the distribution of $Q \to \delta(Q)$, or $\langle Q^2 \rangle / V \to 0$, so the $\theta$ term effectively vanishes.
The quenched approximation of lattice QCD

Quenched approximation: set

\[ \det[\mathcal{D}(m)] = 1 \]

(amounts to omitting quark vacuum polarization to all orders)

For small \( \theta \),

\[ \det [\mathcal{D}(m) + i\theta m \gamma_5] = \det[\mathcal{D}(m)] [1+i\theta m \text{tr}(\gamma_5 \mathcal{D}(m)^{-1}) ] + \mathcal{O}(\theta^2), \]

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

$$\langle p', s' | J^\mu | p, s \rangle_\theta = \bar{u}_{s'}(p') \Gamma^\mu(q^2) u_s(p)$$

$$\Gamma^\mu(q^2) = \gamma^\mu F_1(q^2) + i \sigma^{\mu\nu} q_\nu \frac{F_2(q^2)}{2m}$$

$$+ \left( \gamma^\mu \gamma^5 q^2 - 2m \gamma^5 q^\mu \right) F_A(q^2) + \sigma^{\mu\nu} q_\nu \gamma^5 \frac{F_3(q^2)}{2m}$$

$$J^\mu = \frac{2}{3} \bar{u} \gamma^\mu u - \frac{1}{6} \bar{d} \gamma^\mu d$$

$$J^\mu_V = \bar{u} \gamma^\mu u - \bar{d} \gamma^\mu d$$

$$J^\mu_S = \bar{u} \gamma^\mu u + \bar{d} \gamma^\mu d.$$
The most general matrix element consistent with Lorentz, gauge, CPT symmetries of QCD. The insertion of $J^\mu$ 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

\[
G(t, t') = \langle \chi_N(t', \vec{p}') J^\mu(t, q) \chi_N^\dagger(0, \vec{p}) \rangle
\]

\[
= \sum_{s, s'} \langle 0 | \chi_N | p', s' \rangle \langle p', s' | J^\mu | p, s \rangle \langle p, s | \chi_N^\dagger | 0 \rangle \frac{1}{2E 2E'} e^{-(t'-t)E'} e^{-tE} 
\]

\[
= G^\mu(q) \ast f(t, t', E, E') + \ldots 
\]
With suitable choices of *projectors*, form factors can be determined from the correlation functions, *e.g.* for $\theta = 0$,

\[
\mathcal{P}^{xy} = \frac{i}{4} \frac{1 + \gamma^4}{2} \gamma^x \gamma^y
\]

\[
\mathcal{P}^4 = \frac{11 + \gamma^4}{4} \gamma^4
\]

\[
= \frac{11 + \gamma^4}{4} \gamma^4
\]

\[
\text{tr}\mathcal{P}^{xy} G^{x,y}(q^2) = \pm p_{y,x} m (F_1(q^2) + F_2(q^2))
\]

\[
\text{tr}\mathcal{P}^4 G^4(q^2) = m (E + m) \left( F_1(q^2) + \frac{q^2}{(2m)^2} F_2(q^2) \right)
\]

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.,

\[
\lim_{t' \gg t \gg 0} \frac{1}{p_y} \frac{1}{\text{Tr}P^4 G^4_P(t, t', E, \vec{p})} \frac{\text{Tr}P^{xy} G^x_{P,N}(t, t', E, \vec{p})}{\text{Tr}P^{xy} G^x_{P,N}(q^2)} = \frac{1}{p_y} \frac{\text{Tr}P^{xy} G^x_{P,N}(q^2)}{\text{Tr}P^4 G^4_P(q^2)} = \frac{1}{E + m} \frac{F_1(q^2) + F_2(q^2)}{G^{(P)}_E(q^2)}
\]

\[
\lim_{q \to 0} = \frac{1}{2m} \left\{ 1 + a_{\mu,P} \right\} a_{\mu,N}
\]

yields the magnetic dipole moments

\[F_1(0) = 1, 0\] for the proton, neutron
The physical neutron in the CP-broken vacuum is a mixture of the $\theta = 0$ vacuum (opposite parity) eigenstates $|N\rangle$ and $|N^*\rangle$.

$$|N^\theta\rangle = |N\rangle + i\alpha'|N^*\rangle$$

$\alpha' \propto \theta$

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.

$$\text{tr} \mathcal{P}^{xy} G^z(q^2) = \alpha m(E - m) F_1 + \alpha (m(E - m) + \frac{p_z^2}{2}) F_2 + \frac{p_z^2}{2} F_3 + \mathcal{O}(\theta^2)$$

$$\text{tr} \mathcal{P}^{xy} G^t(q^2) = i p_z \left( \alpha m F_1(q^2) + \alpha \frac{E + 3m}{2} F_2(q^2) + \frac{E + m}{2} F_3(q^2) \right) + \mathcal{O}(\theta^2).$$

The terms proportional to $\alpha$ must be subtracted

$$\lim_{q^2 \to 0} \left\{ \frac{1}{ip_z} \text{tr} \mathcal{P}^{xy} G^t_N(t, t', E, \vec{p}) - \frac{\alpha m F_1(q^2) + \frac{E + 3m}{2} F_2(q^2)}{m(E + m) G_E^{(P)}(q^2)} \right\} = \frac{F_3(q^2)}{2m G_E^{(P)}(q^2)} = \frac{F_3(0)}{2m} = d_N$$
Mixing angle $\alpha$ is calculated from the ratio of two-point functions

[Aoki, Kikukawa, Kuramashi, and Shintani (2004)]

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

To lowest order in $\alpha$ ($\theta$) we have

$$
\text{tr} \frac{1 + \gamma^4}{2} \gamma_5 \quad \langle \chi_{N\theta}(t) \chi_{N\theta}^\dagger(0) \rangle_{\theta} \approx i Z_N \alpha e^{-m_N t}
$$

$$
\text{tr} \frac{1 + \gamma^4}{2} \quad \langle \chi_{N\theta}(t) \chi_{N\theta}^\dagger(0) \rangle_{\theta} \approx Z_N e^{-m_N t}
$$

$$
m_{N\theta} = m_N + O(\theta^2)
$$

$$
Z_{N\theta} = Z_N + O(\theta^2)
$$
Computing with $\theta \neq 0$

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

Assuming $\theta \ll 1$

\[
\approx \frac{1}{Z(0)} \int D\! A_\mu \bar{\psi} D\! \psi (1 - i\theta Q) \mathcal{O} e^{-S(A_\mu)}
\]

\[
= \langle \mathcal{O} \rangle - i\theta \langle Q\mathcal{O} \rangle
\]

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 $a \to 0$. 

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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 $Q \neq 0$

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

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

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

- In large $N$, $\langle OQ \rangle = \langle Q^2 \rangle \frac{\partial \langle O \rangle}{\partial Q} \bigg|_{\nu=0} = \langle Q^2 \rangle \langle O \rangle_{\nu=1}$ [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, $\vec{p} = (\pm 1, 0, 0), (\pm 1, \pm 1, 0), (\pm 1, \pm 1, \pm 1)$ (and permutations) since form factors multiplied by $q^\nu$
  $(\partial/\partial(q^2)|_0$ not accessible on a finite lattice [Wilcox (2002)])
Topological charge “history” (distribution):

\( N_f = 2 \) flavor: small step hybrid monte-carlo, \( Q \) sampled \textbf{slowly}, \textbf{long-time} correlations

Quenched: big change heat bath monte-carlo, \( Q \) sampled \textbf{efficiently}, \( \sim \textbf{no} \) correlations

\( O(a^2) \) improved \( Q \) was computed by integrating the topological charge density after APE smearing the gauge fields.
Topological charge susceptibility $\chi$:

\[
\chi = \frac{\langle Q^2 \rangle}{V} = f^2 m^2 / 8
\]

Statistical errors may be under-estimated (blocks of 50 trajecs)
The mixing coefficient $\alpha$

To lowest order in $\theta$, 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 $\alpha$ difficult: fake plateau
mixing coefficient $\alpha$, quenched

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

Plateau is (almost) trustworthy.

$\alpha = 0.21(3)$ is rather large, *c.f.* topological charge susceptibility
Eigo Shintani’s talk: reweighting with $Q$ is non-trivial, but works!
mixing coefficient $\alpha$, $N_f = 2$ again

Extract $\alpha$ 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 $G_M(q^2)/G^{(P)}_E(q^2)$

$q^2$ dependence mild

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

Anomalous $\mu$'s are equal and opposite well within errors, implies iso-scalar contribution $\sim 0$; 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, $\sim 0$
The ratio of form factors $F_3(q^2)/(2mG_E^{(P)}(q^2))$ is given by:

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

Our conventions have lead to a **positive** central value of $d_{N}/\theta$. Could change as calculation improves.

In physical units,

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

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

Quenched calculation avoids this problem, but $\chi$ 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 $\chi_{\text{PT}}$ 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
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