Lattice QCD and Searches for Violations of Fundamental symmetries

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Baryogenesis and Broken Symmetries

[A.Sakharov (1967)] :

Three necessary conditions:

Why does Universe have More Matter than Antimatter?

$$\frac{n_B - n_{\bar{B}}}{n_{\gamma}} \approx 6 \cdot 10^{-10}$$





(alternatively: leptogenesis + sphalerons)

neutrinoless beta-decays

proton decay, neutron oscillations

Baryon

number-changing

interactions

Violations of C- and CP-

symmetries

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(electric dipole moments of p, n, e⁻, nuclei, atoms)

Interactions out of equlibrium

t | s | 10^{13} 10^{3} 101111111 QCD phase EW phase transition transition Leptogenesis WIMP Big Bang Nucleosynthesis Gravitinos freeze-out Gravitational T_{\min} 10^{-10} 10^{-5} T [GeV]

Lattice QCD and Fundamental Symmetries

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Baryogenesis and Broken Symmetries

Why does Universe have More Matter than Antimatter?



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Primordial

Primordial

Does the Proton Decay?

Missing piece of Grand-Unified Theories Limit on nuclear matter stability





Soudan



Super Kamiokande

- Expected x10 improvement on lifetime limit from Hyper-K, DUNE
- Better sensitivity to $p \rightarrow \overline{\nu}K^+$ that affects supersymmetric GUT models

Proton Decays and Grand Unification



 $\langle \bar{\ell}(q)\Pi(p)|\mathcal{O}^{\chi'}|N(k)\rangle = \bar{v}_{\ell\alpha}^C(q) P_{\chi'} \left[W_0(-q^2) - \frac{i\not q}{m_N} W_1(-q^2) \right] u_N(k)$

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Protons Stable due to Topology?

Why NO proton decay seen ?

- more complicated GUT scenario ?
- other BNV mechanism ?
- small decay amplitude due to nucleon structure ?

"quark pudding" (vac estimate:



 $\langle \operatorname{vac} | \mathcal{O}^{3q} | N \rangle \sim \rho_q^{3/2} \sqrt{V_N} \sim \frac{1}{V_N} \approx 0.004 \, \mathrm{GeV}^3$ $\langle \Pi | \mathcal{O}^{3q} | N \rangle \sim \langle \operatorname{vac} | \mathcal{O}^{3q} | N \rangle / f_\pi \approx 0.03 \, \mathrm{GeV}^2$

However, if the proton is a "Chiral Bag" [A.Martin, G.Stavenga '12]

 proton decay ≡ quantum tunneling of skyrmion over topological barrier

decay rate sensitive to R_{Bag} , quark masses; may be suppressed ~ $O(10^{-4}) - O(10^{-12})$



Uncertainty can be addressed only by a realistic ab initio QCD calculation

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Hadron Correlators in Lattice QCD

Quarks and gluons on a Lattice

- 4D Euclidean space
- discretized action
- controllable extrapolations $a \rightarrow 0, m_{quark} \rightarrow physical$



Observables from correlators of proton=(ud)u, 3-quark decay operators, etc

 $\langle q_x \bar{q}_y \ldots \rangle = \int \mathcal{D} \left(Glue \right) \int \mathcal{D} \left(Quarks \right) e^{-S_{Glue} - \bar{q} \left(\not D + m \right) q} \left[q_x \bar{q}_y \ldots \right]$



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Proton Decay Amplitudes with Physical Quarks



NO SUPPRESSION at physical quark masses \implies Protons sensitive to BNV from GUT

Δ (N_{Baryon})=2 Violation : $n \leftrightarrow \overline{n}$ Oscillations





• $n \leftrightarrow \overline{n}$ oscillation in nuclei : suppressed by interaction $\Delta M \sim O(100 \,\mathrm{MeV})$

n↔**n** Oscillations: Experimental Status



 $\tau_{n\bar{n}} \gtrsim 10^8 \, s$ $\delta m \lesssim 6 \cdot 10^{-24} \, \mathrm{eV}$





• τ (⁵⁶*Fe*) ≥ 0.72·10³² yr

 $\implies \tau_{N\bar{N}} \gtrsim 1.4 \cdot 10^8 \text{ s} [\text{Soudan}]$

- $\tau(^{16}O) \ge 1.77 \cdot 10^{32} \text{ yr}$
 - $\implies \tau_{N\bar{N}} \gtrsim 3.3 \cdot 10^8 \text{ s}$ [Super-K]
- τ (²*H*) ≈ 0.54·10³² yr
 - $\implies \tau_{N\bar{N}} \gtrsim 1.96 \cdot 10^8 \text{ s}$ [SNO]

Nuclear decays from ($\Delta B=2$) transitions: suppressed by nuclear medium:

 $T_d = R\tau_{n\bar{n}}^2$ $R \sim 10^{23} \, \text{s}^{-1}$

nuclear model uncertainty ~ 10-15% for ¹⁶O [E.Friedman, A.Gal (2008)]







SoudanSuper KamiokandeSNOSensitivity is limited by atmospheric neutrinos

$\mathbf{n} \leftrightarrow \overline{\mathbf{n}}$ Amplitudes from Lattice QCD



Lattice calculations at the physical point

[E.Rinaldi, S.S., M.Wagman; PRL'19; PRD'19]



Control of systematic uncertainties

- Chiral-symmetric fermions with physical pion masses
- Variational analysis of ground/excited states



Lattice calculations at the physical point

[E.Rinaldi, S.S., M.Wagman; PRL'19; PRD'19]

	$\mathcal{O}^{\overline{MS}(2 { m GeV})}$	Bag "A"	$\frac{LQCD}{Bag "A"}$	Bag "B"	$\frac{\text{LQCD}}{\text{Bag "B"}}$
$\boxed{[(RRR)_{3}]}$	0	0	_	0	_
$\boxed{[(RRR)_{1}]}$	45.4(5.6)	8.190	$\left(\begin{array}{c} 5.5 \end{array}\right)$	6.660	6.8
$[R_1(LL)_0]$	44.0(4.1)	7.230	6.1	6.090	7.2
$[(RR)_{1}L_{0}]$	-66.6(7.7)	-9.540	7.0	-8.160	8.1
$[(RR)_2 L_1]^{(1)}$	-2.12(26)	1.260	-1.7	-0.666	3.2
$[(RR)_2 L_1]^{(2)}$	0.531(64)	-0.314	-1.7	0.167	3.2
$[(RR)_2 L_1]^{(3)}$	-1.06(13)	0.630	-1.7	-0.330	3.2
	$[10^{-5} \mathrm{GeV}^{-6}]$	$[10^{-5}\mathrm{GeV}^{-6}]$]	$[10^{-5}{\rm GeV}^{-6}]$	

(comparison to MIT Bag model calculations [S.Rao, R.Shrock, PLB116:238 (1982)])

x(5-10) larger N-Nbar oscillation than previously expected

 \implies Stronger constraints on BNV models;

 \implies Great motivation for new $n \leftrightarrow \overline{n}$ experiments

(Next steps:

- "crossed" 2-neutron annihilation amplitudes $\langle vac|O^{6q}|nn \rangle$
- Nuclear medium effects)

n↔n Oscillations: Experimental Outlook



Maximize Probability of oscillation ~ N_n ($T_{\rm free}$)²

- Shielded beam (similar to ILL): Expected sensitivity x10²-10³ ILL τ_{n-π} ≥10⁹-10¹⁰ s
 ◆ Spallation sources: x12 flux @ESS
 - Elliptic focussing mirror
 - Better magnetic shielding (B < 1 nT)

[Phillips et al, arXiv:1410.1100]



stored ultra-cold neutrons $\tau_{n-\overline{n}} \gtrsim 2.2 \cdot 10^8 \text{ s}$



- Further improvements
 - Larger vessels
 - Better magnetic shielding (B < 1 nT)</p>
 - Parabolic floor concentrators
 - Multiple coherent reflections

CP Violation & Neutron Electric Dipole Moment



$$\vec{d}_N = d_N \frac{\vec{S}}{S}$$

 $\mathcal{H} = -\vec{d}_N \cdot \vec{E}$





Magnetic dipole moment $\vec{\mu}_n = \mu_n \vec{S}$

Electric dipole moment $\vec{d_n} = d_n \vec{S}$

EDMs are the most sensitive probes of CPv:

- Signals for beyond SM physics
 - (SM = 10⁻⁵ of the current exp.bound)
- Prerequisite for Baryogenesis
- Strong CP problem : θ_{QCD}-induced EDM?



Experimental Outlook

Current nEDM limits:

|d_n| < 2.9 × 10⁻²⁶ e ⋅ cm (stored UC neutrons)
 [Baker et al, PRL97: 131801(2006)]
 |d_n| < 1.6 × 10⁻²⁶ e ⋅ cm (¹⁹⁹Hg)
 [Graner et al, PRL116:161601(2016)]

Future nEDM sensitivity :

- 1–2 years : next best limit?
- 3–4 years : x10 improvement
- 7-10 years : x100 improvement

	10 ⁻²⁸ e cm
CURRENT LIMIT	<300
Spallation Source @ORNL	< 5
Ultracold Neutrons @LANL	~30
PSI EDM	<50 (I), <5 (II)
ILL PNPI	<10
Munich FRMII	< 5
RCMP TRIUMF	<50 (I), <5 (II)
JPARC	< 5
Standard Model (CKM)	< 0.001

[Snowmass EDM workshop report, arXiv:2203.08103]



Electric Dipole Moments: Window to New Physics



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Determination of Nucleon EDM

 Compute *Energy Shift* in uniform electric field [S.Aoki et al '89 ; E.Shintani et al '06; E.Shintani et al, PRD75, 034507(2007)]

$$\langle N(t)\bar{N}(0)\rangle_{\theta,\vec{E}} \sim e^{-(E\pm\vec{d}_N\cdot\vec{E})t}$$

• Compute *CPv Form-Factor* F_3 : $d_N = F_3(Q^2 \rightarrow 0) / (2m_N)$ [(everybody else, almost)]

 $\langle N_{p'} | \bar{q} \gamma^{\mu} q | N_p \rangle_{\mathcal{CP}} = \bar{u}_{p'} \Big[F_1 \gamma^{\mu} + (F_2 + i F_3 \gamma_5) \frac{i \sigma^{\mu\nu} (p' - p)_{\nu}}{2m_N} \Big] u_p$

- pre-2017 : spurious $\mu_n \leftrightarrow d_n$ mixing
- Dragos et al(2019)
- Alexandrou et al(2020)
- Bhattacharya et al (2021)
- Liang et al (2023)

 $d_n / \theta = -0.0015(7) \ e \cdot \text{fm}$ $d_n / \theta = -0.0009(24) \ e \cdot \text{fm}$

- $|d_n / \theta| \lesssim 0.01 \ e \cdot \mathrm{fm}$
- $d_n / \theta = -0.0015(1)(3) e \cdot \text{fm}$





Nucleon "Parity Mixing"

CPv interaction induces a chiral phase in nucleon spinor ; lattice calculations of EDM have to account for that [M.Abramczyk, S.Aoki, S.N.S, et al (2017) arXiv:1701.07792]

 $\langle \operatorname{vac}|N|p,\sigma \rangle_{\mathcal{CP}} = e^{i\alpha\gamma_5} u_{p,\sigma} = \tilde{u}_{p,\sigma}$

Value of α -mixing is critical for correct determination of EDM:

$$F_3^{\text{lat}}(Q^2) \approx \frac{m}{q_3} \underbrace{\langle N_{\uparrow}(0) | \bar{q}\gamma_4 q | N_{\uparrow}(-q_3) \rangle_{\mathcal{CP}}}_{\mathcal{CP}} - \underbrace{\alpha_5 G_E(Q^2)}_{\mathcal{CP}}$$

CPv matrix element

Sachs form factor subtraction



Pre-2017 lattice results for θ_{QCD} -*n*EDM: *original* and *corrected*

		$m_{\pi} [{ m MeV}]$	$m_N [{ m GeV}]$	$ ilde{F}_3$	F_3
[ETMC 2016]	n	373	1.216(4)	-0.555(74)	0.094(74)
[Shintani et al 2005]	n	530	1.334(8)	-0.325(68)	-0.048(68)
	p	530	1.334(8)	0.284(81)	0.087(81)
[Berruto et al 2006]	n	690	1.575(9)	-1.39(1.52)	-1.15(1.52)
	n	605	1.470(9)	0.60(2.98)	1.14(2.98)
	n	465	1.246(7)	-0.375(48)	-0.130(76)
	n	360	1.138(13)	-0.248(29)	0.020(58)

Nucleon "Parity Mixing"

CPv interaction induces a chiral phase in nucleon spinor ; lattice calculations of EDM have to account for that [M.Abramczyk, S.Aoki, S.N.S, et al (2017) arXiv:1701.07792]

 $\langle \operatorname{vac}|N|p,\sigma \rangle_{\mathcal{GP}} = e^{i\alpha\gamma_5} u_{p,\sigma} = \tilde{u}_{p,\sigma}$

Value of α-mixing is critical for correct determination of EDM:

$$F_3^{\text{lat}}(Q^2) \approx \frac{m}{q_3} \underbrace{\langle N_{\uparrow}(0) | \bar{q}\gamma_4 q | N_{\uparrow}(-q_3) \rangle_{\text{CP}}}_{\text{QP}} - \underbrace{\alpha_5 G_E(Q^2)}_{\text{QP}}$$

CPv matrix element

Sachs form factor subtraction

- Proton ($G_{Ep}(0)=1$) : Correction ~ α_5
- Neutron (G_{En}(0)=0) : No correction at Q²=0 However, Q²→0 extrapolation may be skewed by neutron electric form factor ~α₅ G_{En}(Q²)



Signal & Noise in θ_{QCD} -induced nEDM





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Alternative: Background Electric Field



Calculation of magnetic and electric moments, hadron polarizabilities [W.Detmold et al (2009)]

Electric field on a periodic lattice is "quantized"

$$\mathcal{E}_{\min} = \frac{1}{|q_d|} \frac{2\pi}{L_x L_t}$$
$$\approx 0.037 \,\text{GeV}^2 = 187 \,\text{MV/fm}$$

for a $(2.8 \text{ fm})^3 x (5.6 \text{ fm})$ lattice

Feynman-Hellman theorem : relate energy shift ...

$$m'_N = m_N - (d_N^{\theta} \theta) \, \vec{\Sigma} \cdot \vec{\mathcal{E}}$$

... to matrix element of local topological charge density



polarized in spin and charge

Advantages:

- sample GG only on one time slice
 moise reduction
- no need for $Q^2 \rightarrow 0$ momentum extrapolation

Topological Charge with Gradient Flow

Gradient flow: covariant *4D-diffusion* of quantum fields with "G.F." time t_{GF} :

Tree-level:

Gradient-flowed topological charge:

total top. charge on 20 randomly



$$\begin{bmatrix} \text{M.Luscher, JHEP08:071; 1006.4518]} \\ \frac{d}{dt_{\text{GF}}} B_{\mu}(t_{\text{GF}}) = D_{\mu}G_{\mu\nu}(t_{\text{GF}}), \quad B_{\mu}(0) = A_{\mu} \\ B_{\mu}(x, t_{\text{GF}}) \propto \int d^{4}y \exp\left[-\frac{(x-y)^{2}}{4t_{\text{GF}}}\right] A_{\mu}(y) \\ \tilde{Q}(t_{\text{GF}}) = \int d^{4}x \frac{g^{2}}{32\pi^{2}} \left[G_{\mu\nu}\tilde{G}_{\mu\nu}\right]\Big|_{t_{\text{GF}}} \end{aligned}$$

- continuous "cooling": effective scale $\Lambda_{\rm UV} \rightarrow (t_{\rm GF})^{-1/2}$
- smoothing fields (reduce |Gµν|)
 remove Gµν dislocations;
 dynamical separation of top. sectors
 [M.Luscher, JHEP08:071; 1006.4518]
- "diffusion" of topological charge density makes it nonlocal

Gradient-Flowed Topological Charge Density



$$24^3 \times 64$$
 lattice, $m\pi \approx 340 \ MeV$

$$q(x) = \frac{g^2}{32\pi^2} G^a_{\mu\nu} \widetilde{G}^a_{\mu\nu}$$
$$\approx \frac{1}{16\pi^2} \frac{1}{a^4} \operatorname{Tr} \left[G^{\text{lat}}_{\mu\nu} \widetilde{G}^{\text{lat}}_{\mu\nu} \right]$$
$$\propto (\mathbf{E} \cdot \mathbf{H})_{\text{color}}$$

Instantons and Anti-Instantons : Quantum tunneling of gluon field between topological sectors



 $\mathsf{CPv}\text{-}\mathsf{QCD}\ \boldsymbol{\varTheta}\text{-}\mathsf{Vacuum}:$

$$|vac\rangle_{\theta} = \sum_{Q} e^{i\theta Q} |Q\rangle$$

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Tunneling Between Topology Sectors



$$q(x) = \frac{g^2}{32\pi^2} G^a_{\mu\nu} \widetilde{G}^a_{\mu\nu}$$
$$\approx \frac{1}{16\pi^2} \frac{1}{a^4} \operatorname{Tr} \left[G^{\text{lat}}_{\mu\nu} \widetilde{G}^{\text{lat}}_{\mu\nu} \right]$$
$$\propto (\mathbf{E} \cdot \mathbf{H})_{\text{color}}$$

Instantons and Anti-Instantons : Quantum tunneling of gluon field between topological sectors



CPv-QCD Θ -Vacuum :

$$|vac\rangle_{\theta} = \sum_{Q} e^{i\theta Q} |Q\rangle$$

Extrapolation to the Physical Point



Summary

- Nucleon structure calculations on a lattice are critical to searches for symmetry violations, understanding the origin of nuclear matter
 - Proton decays $p \rightarrow \pi/K$, $p \rightarrow leptons$

No topological suppression of nucleon decay found; confirm limits on GUTs NEXT: $p \rightarrow \rho \rightarrow \pi \pi$, $p \rightarrow K^* \rightarrow \pi K$ amplitudes

Neutron-antineutron oscillation Amplitudes × (6 ... 8) larger than from pheno.models NEXT: $nn \rightarrow vacuum$ amplitudes, $n \rightarrow \overline{n}$ in nuclear medium

Novel method to compute nEDM from local topological charge Cross-check for electric-dipole form factor calculation Results consistent with earlier works Potential method of choice for physical-point calculations with large V₄ BACKUP

BACKUP

Proton Decay : Extrap. in Q² and Lattice Spacing



Searches for N \Leftrightarrow \overline{N} in Nuclei



Nucleus decay from (nn) annihilation

 $T_d = R\tau_{n\bar{n}}^2 \qquad r$

 $R \sim 10^{23} \, s^{-1}$

Nuclear medium effect suppresses

neutron/antineutron oscillation

nuclear model uncertainty ~ 10-15% for ¹⁶O [E.Friedman, A.Gal (2008)]



Sensitivity is limited by atmospheric neutrinos



Soudan

Super Kamiokande





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 $\Delta M \sim 100 \text{ MeV}$

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Matrix Elements of GG (Low-mode Improved)



Two effects observed: 1. Convergence to ground state matrix el. 2. Diffusion of top.charge for $t_{sep} \leq 7a$

PRELIMINARY estimates $2md_n = F_3(0) \approx 0.11 \dots 0.13$ **agree with form factor**

Analysis of (τ_Q, t_{GF}) required to detangle $\langle N | G \widetilde{G} | N \rangle$, $\langle N | G \widetilde{G} | N \rangle_{exc}$, $\langle vac | G \widetilde{G} | N \overline{N} \rangle$,

. . .