Perspectives on the strong CP problem

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Why is it assumed that there is a Strong CP Problem?

The most general renormalizable QCD Lagrangian density allowed by the usual local symmetries can be written as

$$\mathcal{L}_{\rm QCD} = \mathcal{L}_{\rm min} + \theta q(x) = -\tfrac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(i \not{D} - M)\psi + \theta\, q(x), \quad q(x) = \tfrac{g^2}{32\pi^2} F^a_{\mu\nu} \widetilde{F}^{a\mu\nu}. \tag{1}$$

- $q(x)$ is a local, gauge-invariant, dimension-four pseudoscalar operator.
- The term $\theta q(x)$ is therefore compatible with locality, Lorentz invariance, gauge invariance, and renormalizability.
- $q(x)$ is odd under P and CP $\Rightarrow$ $\theta \neq 0$ appears to allow strong-interaction CP violation.
- The axial anomaly $\Rightarrow$ a gluonic θ term and a flavor-singlet pseudoscalar quark mass term can be transformed into one another, so that only the combination $\bar{\theta}$ is physically relevant:

$$\boxed{\bar{\theta} = \theta + \arg\det M}. \tag{2}$$

This talk summarizes the arguments in Refs. [1, 2].

But where is strong CP violation?

There is presently no experimental evidence for strong-interaction *CP* violation.

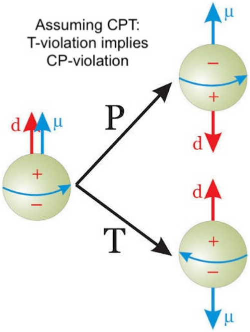
Assuming *CPT*: *T* violation $\Leftrightarrow$ *CP* violation.

The most sensitive constraint comes from searches for the neutron electric dipole moment:

$$\textit{Theory}: \quad d_n(\bar\theta) \sim 10^{-16}\,\bar\theta\ e\,\mathrm{cm}, \tag{3}$$

$$\textit{Experiment}: \quad |d_n|_{\mathrm{exp}} \lesssim 10^{-26}\ e\,\mathrm{cm}, \tag{4}$$

$$\Rightarrow \quad \boxed{|\bar\theta| \lesssim 10^{-10}} \tag{5}$$



- *Strong CP problem*: Why should a parameter naively of $\mathcal{O}(1)$ be fine-tuned to $\lesssim 10^{-10}$?

A logically prior question:

What requires $\bar\theta$ to be an independent physical parameter of QCD in the first place?

The answer is not straightforward.

Minimal QCD: Start with the local theory

Start with the established local structure of QCD, without introducing an independent physical flavor-singlet *CP*-violating parameter or any additional global topological classification:

$$\boxed{\mathcal{L}_{\min} = -\tfrac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(i\not{D} - M)\psi} \tag{6}$$

where the quark masses are chosen *real* and *positive*.

- This is a local, Lorentz-invariant, gauge-invariant and renormalizable quantum field theory.
- It contains the full local and nonperturbative gauge dynamics of QCD.
- In particular, the local gauge-invariant operator

$$\boxed{q(x) = \frac{g^2}{32\pi^2} F^a_{\mu\nu} \widetilde{F}^{a\mu\nu}} \equiv \text{topological charge density} \tag{7}$$

  is still present in the theory – *but* no independent *physical* θ term, $\theta q(x)$, or flavor-singlet pseudoscalar quark mass term has been introduced. Thus $\mathcal{L}_{\min}$ contains no $\bar{\theta}$ parameter.
- The axial anomaly and its Ward identities all follow in the usual way.
- For convenience we will refer to this starting point *minimal QCD*.

Minimal QCD assumes nothing about global integer-valued topological classification.

Minimal QCD: The Axial Anomaly is a local relation

The flavor-singlet axial current satisfies the anomalous Ward identity

$$\boxed{\partial_\mu J_5^\mu = 2i\,\bar{\psi} M \gamma_5 \psi + 2N_f\, q(x)}, \qquad \text{where} \quad q(x) = \frac{g^2}{32\pi^2} F^a_{\mu\nu} \widetilde{F}^{a\mu\nu}. \tag{8}$$

- The anomaly is a *local* operator relation.
- It is present in minimal QCD even though no physical θ parameter has been introduced.
- Hence the anomalous $U(1)_A$ physics associated with $q(x)$ has not disappeared.
- Nonperturbative fluctuations of $q(x)$ are characterized by its correlation functions, in particular the topological susceptibility χ,

$$\boxed{\chi = \int d^4x_E\, \langle q(x_E) q(0) \rangle_E}, \qquad \text{where } E \text{ denotes Euclidean space.} \tag{9}$$

$q(x)$ remains a nontrivial local operator with physically important correlation functions, independent of the existence or otherwise of a physical $\bar{\theta}$ term.

Minimal QCD: topological susceptibility without a physical $\bar{\theta}$

At $\bar{\theta} = 0$, CP symmetry gives

$$\langle Q \rangle = 0, \qquad \text{where} \qquad Q \equiv \int d^4x_E\, q(x_E). \tag{10}$$

Conventionally Q is referred to as the *topological charge*, but no configuration-by-configuration integer-valued interpretation of Q is assumed here. Fluctuations of the local density give

$$\langle Q^2 \rangle = \int d^4x_E\, d^4y_E\, \langle q(x_E) q(y_E) \rangle_E, \tag{11}$$

$$\chi = \lim_{V_4 \to \infty} \langle Q^2 \rangle / V_4 = \int d^4x_E\, \langle q(x_E) q(0) \rangle_E. \tag{12}$$

- Thus $\theta = 0$ does *not* imply $q(x) = 0$ or the absence of topological charge-density fluctuations.
- Introduce, if desired, an auxiliary *source parameter* θ:

$$Z_E(\theta) = \int \mathcal{D}\Phi \, \exp\left[-S_E + i\theta \int d^4x_E\, q(x_E) \right] \qquad \Rightarrow \qquad \chi = -\frac{1}{V_4} \left. \frac{\partial^2 \ln Z_E(\theta)}{\partial \theta^2} \right|_{\theta=0}. \tag{13}$$

The use of source term to generate correlation functions and then setting the source to zero is useful, but it is <u>not</u> the introduction of a physical $\bar{\theta}$ term.

Minimal QCD: Witten–Veneziano and Leutwyler–Smilga relations

Important anomalous and chiral QCD phenomenology follows from the local anomaly, topological charge-density correlations and the appropriate low-energy and large-N_c expansions.

Witten–Veneziano

For three light flavors,

$$\boxed{m_{\eta'}^2 + m_\eta^2 - 2m_K^2 = (2N_f/f_0^2)\chi_{\mathrm{YM}} + \cdots} \quad (14)$$

where $\chi_{\mathrm{YM}} = \int d^4x_E \, \langle q(x_E)q(0)\rangle_{\mathrm{YM}}$. (15)

- $\chi_{\mathrm{YM}} \equiv$ *pure Yang–Mills* susceptibility.
- Uses the anomalous Ward identity, chiral dynamics and large-N_c.
- Accounts for the anomalously large η' mass.

Leutwyler–Smilga

Define $\Sigma \equiv -\langle \bar{q}q\rangle_{m=0}$. For light quarks,

$$\boxed{\chi = \Sigma\bar{m} + O(m^2) = \frac{\Sigma}{\sum_{f=1}^{N_f} \frac{1}{m_f}} + O(m^2)}, \quad (16)$$

where $1/\bar{m} = \sum_{f=1}^{N_f} \frac{1}{m_f}$. (17)

For N_f degenerate masses,

$$\chi = (m\Sigma/N_f) + O(m^2). \quad (18)$$

- Follows from the anomalous Ward identity and low-energy chiral effective theory.

Neither important relation requires a physical $\bar{\theta}$ or the exact functional integral to be decomposed configuration by configuration into integer-labelled Q sectors.

Minimal QCD and cluster decomposition

Cluster decomposition is a fundamental locality property of QCD: for gauge-invariant local operators separated by a large spacelike distance,

$$\boxed{\langle \mathcal{O}_A(x)\mathcal{O}_B(y)\rangle \longrightarrow \langle \mathcal{O}_A(x)\rangle\langle \mathcal{O}_B(y)\rangle} \qquad |x-y|^2 \to -\infty. \tag{19}$$

- In minimal QCD the functional integral is **not** restricted to configurations with integer Q,

$$\boxed{Q \equiv \int d^4x_E \, q(x_E).} \tag{20}$$

- $\Rightarrow$ no fixed-Q global constraint correlating arbitrarily distant spacetime regions.
- Cluster decomposition is a property of correlation functions of local physical observables; no θ vacuum is needed to remove a fixed-Q restriction that was never introduced.
- *Only* if one first decomposes the functional integral into fixed integer-Q sectors does restriction to a single sector introduce the familiar global constraint relevant to clustering.

The fixed-integer-Q clustering issue does not occur in Minimal QCD. It can only arise after imposing a global Q-sector decomposition of the functional integral.

Minimal QCD still contains instantons

Coarse-grained spacetime observables $\Rightarrow$ Classical & semiclassical physics emerge.
Effective smoothing of rough quantum fields reveals semiclassical physics, e.g., instantons,
Instantons = saddle points in semiclassical expansion of Euclidean functional integral
= smooth finite-action classical solutions of the Euclidean Yang–Mills equations.

$$F_{\mu\nu} = \pm\widetilde{F}_{\mu\nu}, S_{\text{inst}} = 8\pi^2/g^2, \quad (21)$$

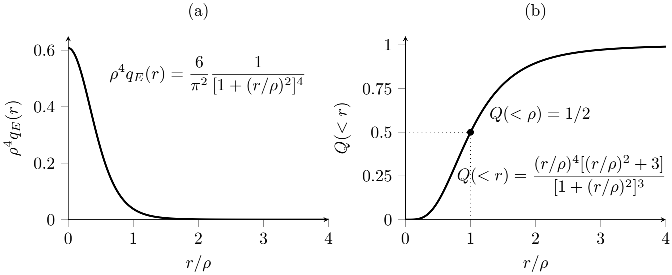
$$Q = \int d^4x_E\, q_E(x) = \pm 1. \quad (22)$$

The BPST instanton solution $Q = 1$,

$$q_E(x) = \frac{6}{\pi^2}\frac{\rho^4}{[(x-x_0)^2+\rho^2]^4}, \quad (23)$$

$$\int d^4x_E\, q_E(x) = 1. \quad (24)$$

- Fermion zero modes & 't Hooft interaction remain



Local density $q_E(r) \to$ integrated charge $Q(r) \xrightarrow{r\to\infty} 1$

Instantons still arise in Minimal QCD in the semiclassical limit and do not require global Q-sector decomposition of the full functional integral.

What does minimal QCD give us?

So far we have made *no assumption* that there is a physical $\bar{\theta}$ or that the functional integral is restricted to gauge-field configurations with integer topological charge Q.

Nevertheless, Minimal QCD contains:

- perturbative and nonperturbative QCD dynamics,
- the axial anomaly and anomalous Ward identities,
- nonzero topological susceptibility,
- Witten–Veneziano and Leutwyler–Smilga relations,
- cluster decomposition,
- instantons and their semiclassical physics.

All known QCD phenomenology appears to follow from Minimal QCD alone.

Additional Global Assumptions: Integer topological charge

Now consider imposing *additional global* regularity and boundary conditions on gauge fields in the Euclidean functional integral:
Assuming sufficiently smooth and finite-action gauge fields A_μ on $\mathbb{R}^4$ we have:,

- Smooth $\Rightarrow Q \equiv \frac{g^2}{32\pi^2} \int d^4x_E \, F^a_{\mu\nu} \widetilde{F}^a_{\mu\nu} \in \mathbb{Z}$, integer topological charge Q.
- Finite action $\Rightarrow F_{\mu\nu} \to 0$ sufficiently rapidly at Euclidean infinity.
- As $|x| \to \infty$ we have $A_\mu(x) \to$ a pure gauge field. This defines a map $U : S^3_\infty \to SU(3)$.
- Such maps U have integer winding number $\nu[U]$:
  U winds S^3 around $SU(3)$ $\nu[U]$ times, where since $\pi_3(SU(3)) = \mathbb{Z}$ then $\nu[U] \in \mathbb{Z}$.
- It can be shown that the topological charge Q is exactly this winding-number $\nu[U]$.
- For a smooth finite-action gauge field A we have $\boxed{Q = \nu[U] \in \mathbb{Z}}$.

$\Rightarrow$ **Smooth finite-action gauge fields A_μ have global topological classification $Q \in \mathbb{Z}$.**

Consequence: Topological sectors in the Euclidean framework

Let $\mathcal{C}$ be the space of sufficiently smooth finite-action gauge fields with integer Q. The space of such gauge fields then separates into integer Q-labelled sectors,

$$\mathcal{C} = \bigcup_{Q\in\mathbb{Z}} \mathcal{C}_Q. \tag{25}$$

If we *assume* that the functional integral contains only smooth finite-action gauge fields, then

$$Z \equiv \int_{\mathcal{C}} \mathcal{D}A\,\mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-S_E} = \sum_{Q=-\infty}^{+\infty} Z_Q, \quad \text{where} \quad Z_Q = \int_{\mathcal{C}_Q} \mathcal{D}A\,\mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-S_E}. \tag{26}$$

- One could in principle assign a different relative weight $w(Q)$ to each Z_Q.
- Requiring all Q sectors to contribute with equal magnitude $\Rightarrow |w(Q)| = 1$.
- For localized fluctuations with charges Q_1, Q_2 in widely separated spacetime regions, cluster decomposition and additivity of $Q \Rightarrow w(Q_1+Q_2) = w(Q_1)w(Q_2)$.
- Therefore $w(Q)$ is a unitary character of $\mathbb{Z}$, $w(Q) = e^{i\theta Q}$ up to a global phase:

$$\Rightarrow \text{We can weight each } Z_Q \text{ with } e^{i\theta Q}: \quad \boxed{Z \to Z(\theta) \equiv \sum_{Q=-\infty}^{+\infty} e^{i\theta Q} Z_Q.} \tag{27}$$

- This is equivalent to adding $-i\theta Q$ to the Euclidean action, and hence

$$\boxed{\mathcal{L}_E(\theta) = \tfrac{1}{4} F^a_{\mu\nu} F_{a\mu\nu} + \bar{\psi}(i\not{D}_E + M)\psi - i\theta q_E} = \textbf{Extended QCD}. \tag{28}$$

Hamiltonian Formulation: Global Assumptions

On a spatial slice $\mathbb{R}^3$, first *restrict* to smooth gauge transformations U and then impose the *additional* restriction that allowable transformations satisfy

$$U(\mathbf{x}) \to U_\infty \text{ for } |\mathbf{x}| \to \infty \;\Rightarrow\; \mathbb{R}^3 \xrightarrow{\text{compactifies}} S^3 \;\Rightarrow\; U : S^3 \to SU(3),\ \pi_3(SU(3)) = \mathbb{Z}. \quad (29)$$

- Gauge transformations are then labelled by an integer winding number n:

$$\textit{small} \text{ gauge transformations: } n = 0; \qquad \textit{large} \text{ gauge transformations: } n \neq 0. \quad (30)$$

- Classical vacua have $F_{ij} = 0$ and so are pure gauge. Acting on the trivial classical vacuum $A_i = 0$ with U_n gives:

$$A_i^{(n)} = (i/g) U_n \partial_i U_n^\dagger, \qquad \boxed{\text{Chern-Simons number} \equiv N_{\mathrm{CS}}[A^{(n)}] = n}. \quad (31)$$

- For smooth Euclidean fields interpolating between asymptotic vacua at $x_4 = \pm\infty$,

$$\boxed{Q = \int d^4x_E\, q_E(x) = \Delta N_{\mathrm{CS}} = N_{\mathrm{CS}}^{\mathrm{final}} - N_{\mathrm{CS}}^{\mathrm{initial}}.} \quad (32)$$

- $Q = \pm 1$ instantons/anti-instantons interpolate semiclassically between neighboring $A_i^{(n)}$, i.e., between neighboring integer-labelled classical vacua .

$$\boxed{\textbf{Smoothness and global restrictions on } U(\mathbf{x}) \Rightarrow \textbf{integer-labelled classical vacua } A_i^{(n)}\textbf{.}}$$

Hamiltonian Formulation: From large gauge transformations to θ

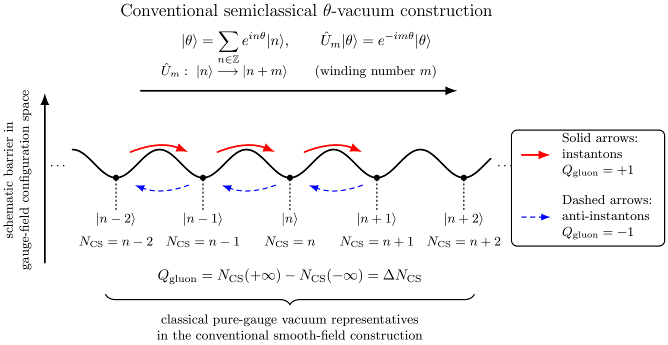
After quantization, Gauss's law is $\hat{G}^a(\mathbf{x})\,|\psi_{\rm phys}\rangle = 0$. *Small* gauge transformations are generated by $\hat{G}^a(\mathbf{x})$, so $|\psi_{\rm phys}\rangle$ are invariant under these.

- Winding numbers add:
$$\hat{U}_m \hat{U}_n = \hat{U}_{m+n}. \tag{33}$$
- Physical states may therefore transform under the 1-dim unitary representations of $\mathbb{Z}$,
$$\boxed{\hat{U}_n\,|\psi_\theta\rangle = e^{-in\theta}\,|\psi_\theta\rangle\,, \qquad \theta \sim \theta + 2\pi.} \tag{34}$$
- Different θ label superselection sectors $\mathcal{H}_\theta$; denote the vacuum in each by $|\theta\rangle$.
- Semiclassically, with $|n\rangle$ associated with the integer-labelled classical vacua,
$$\boxed{|\theta\rangle_{\rm semiclass} = \sum_{n\in\mathbb{Z}} e^{in\theta}\,|n\rangle\,, \qquad \hat{U}_m\,|\theta\rangle_{\rm semiclass} = e^{-im\theta}\,|\theta\rangle_{\rm semiclass}\,.} \tag{35}$$
- So *define* the θ vacuum, $|\theta\rangle_{\rm semiclssical}$, it is invariant under all large gauge transormations.

The global restriction on allowable gauge transformations leads to the θ-labelled quantum theory.

Hamiltonian formulation: The θ vacuum – semiclassical picture

- For brevity write $|\theta_{\text{semiclass}}\rangle$ as $|\theta\rangle$ here.
- Schematic representation of the conventional semiclassical construction of the θ vacuum.
- Classical pure-gauge configurations are represented by minima labelled by their Chern-Simons numbers $N_{\text{CS}} = n$.
- Large spatial gauge transformation of winding number m relates vacuum-type states as $\hat{U}_m\,|n\rangle = |m+n\rangle$.
- Smooth Euclidean instantons and anti-instantons interpolate asymptotic vacua, with $Q = \Delta N_{\text{CS}} = \pm 1$.



- **$|n\rangle \equiv$ semiclassical states related to integer-labelled classical pure-gauge vacua.**
- **Instantons/anti-instantons act between neighboring n-sectors: $Q = \Delta N_{\text{CS}} = \pm 1$.**
- **Physical θ vacua are simultaneous eigenstates of all large gauge transformations:**

$$\boxed{|\theta\rangle = \sum_{n\in\mathbb{Z}} e^{in\theta}\,|n\rangle\,, \qquad \hat{U}_m\,|\theta\rangle = e^{-im\theta}\,|\theta\rangle \quad \text{for all} \quad m \in \mathbb{Z}.} \tag{36}$$

But the full quantum functional integral is *not* semiclassical

The conventional integer-Q construction applies directly subject to having sufficiently smooth finite-action gauge fields. The Hamiltonian approach also restricts the space of allowed gauge transformations ($U(\mathbf{x}) \to \mathbf{U}_\infty$ for all $|\mathbf{x}| \to \infty \;\Rightarrow\;$ all winding on final/initial time surfaces).

- Generic quantum fields are *rough*, not smooth classical configurations, $Q \notin \mathbb{Z}$ [3, 4, 5].
- Asymptotic freedom $\Rightarrow$ short-distance fields approach free-field behaviour – but free quantum fields are themselves distributional/rough [6].
- On the lattice the fundamental variables are independent group-valued links integrated with the Haar measure: generic configurations need not approximate smooth continuum gauge fields. **Taking $a \to 0$ does not make the raw lattice ensembles smooth** [7, 8].
- Gradient/Wilson flow can smooth lattice fields and produce a well-defined near-integer topological charge, but that is an **additional** process not required by Minimal QCD.
- Raw unflowed/unsmoothed quantum field configurations are typically rough and so do not possess a smooth configuration-by-configuration integer Q.

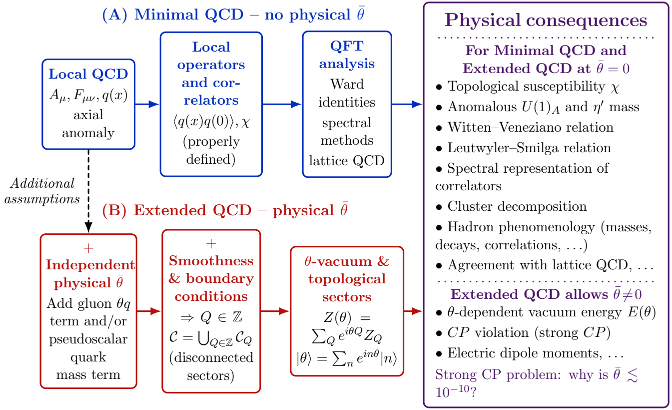
The smooth-field topological classification of the full quantum functional integral is an additional assumption, rather than a consequence of Minimal QCD.

Minimal QCD vs Extended QCD

- **Minimal QCD:** local QCD + anomaly + $q(x)$ correlations + nonperturbative dynamics, with no CP-violating parameter $\bar{\theta}$.
- **Extended QCD:** introduce an independent physical $\bar{\theta}$ parameter as a gluonic θ term, a flavor-singlet pseudoscalar quark mass term, or a combination: $\bar{\theta} = \theta + \arg\det M$.
- **Conventional global construction:** additional global assumptions concerning smoothness, boundary conditions and topology give $Q \in \mathbb{Z}$, θ weighting, θ sectors and the θ vacuum.
- Extended QCD can be introduced *with or without* the conventional global construction that allows an integer-Q decomposition of the full functional integral.

Minimal and Extended QCD

Both formulations are consistent with established $\bar{\theta} = 0$ QCD phenomenology;
The distinction is whether an independent physical $\bar{\theta}$ parameter is introduced.



Minimal and Extended QCD contain the same established QCD physics at $\bar{\theta} = 0$.

Conclusion and foundational question

Extended QCD with a physical $\bar{\theta}$ is mathematically self-consistent. In the conventional global formulation this leads to

$$\bar{\theta} \neq 0, \text{ expect } \bar{\theta} = O(1) \;\Rightarrow\; \text{expect large strong } CP \text{ violation, but } |\bar{\theta}| \lesssim 10^{-10}. \tag{37}$$

But we note that:

- All presently established QCD phenomenology follows from Minimal QCD.
- No known observable has been identified that requires the exact quantum functional integral to possess a configuration-by-configuration integer-Q decomposition.
- The anomaly, susceptibility, WV/LS relations, cluster decomposition, instantons, lattice QCD and hadron phenomenology remain intact in Minimal QCD.

Foundational question: What physical phenomenon or foundational principle requires $\bar{\theta}$ to be an independent physical parameter of QCD, rather than merely allowing it?

If none does, the conventional strong CP problem need not be an unavoidable feature of QCD, but arises only after an independent physical $\bar{\theta}$ parameter is admitted.

What this does *not* imply

This talk only questions the *necessity of the strong CP problem* – not the broader motivation for axion physics, which is independently well motivated.

- Axions [9, 10, 11], axion-like particles (ALPs) [12, 13, 14] and related BSM models [15] arise naturally in many extensions of the Standard Model.
- They have rich possible implications for particle physics, astrophysics and cosmology [16, 17, 18].
- They are compelling dark-matter candidates $\Rightarrow$ extensive and important experimental search programs [13, 16, 17, 18].
- These motivations exist *independently* of whether the conventional strong CP problem is an unavoidable feature of QCD.

$$\boxed{\textbf{Questioning strong CP} \neq \textbf{questioning axion/ALP physics.}}$$

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Backup slides

Yes, but "Shouldn't every allowed operator be included"?

A common argument is: if a local operator is allowed by the symmetries, its coefficient should be regarded as an *independent physical* parameter.

[Ed Witten: $\bar{\theta}$ is allowed and there is no known reason for it not to be there $\Rightarrow$ the strong CP problem]

- For ordinary operators this is often required by operator mixing arising from renormalization. For example, in a Yukawa theory a ϕ^4 counterterm is needed for renormalization and so a physical ϕ^4 term *must* be introduced to close the theory:

$$\mathcal{L}_{\mathrm{ren}} \supset -g\,\bar{\psi}\phi\psi - \lambda\phi^4 + \cdots \,. \tag{38}$$

- The topological density is a total four-divergence: $q(x) = [g^2/(32\pi^2)] F^a_{\mu\nu}\widetilde{F}^{a\mu\nu} = \partial_\mu K^\mu$.
  $\Rightarrow$ For constant θ and an arbitrary field variation of compact support,

$$\boxed{\delta\left[\theta \int d^4x\, q(x)\right] = \theta \int d^4x\, \partial_\mu \delta K^\mu = 0.} \tag{39}$$

  Thus the constant θ term produces no *local* variational response and so is an *unusual operator* in nature. It does not mix with other QCD operators under renormalization.

The question is not "what forbids such an operator"?. The real question is "what requires such an operator"? Our discussion asks the second question.

What does a recent lattice calculation of d_n actually show?

A recent lattice calculation [19] started from CP-conserving lattice QCD at $\bar{\theta} = 0$. They then calculated the linear response of a lattice calculation of the neutron EDM to a $\bar{\theta}$ *source term*:

- Linear response gives

$$d_n(\bar{\theta}) = \bar{\theta} \left. \frac{\partial d_n}{\partial \bar{\theta}} \right|_{\theta=0} + O(\bar{\theta}^3). \tag{40}$$

- Their recent lattice result is

$$\boxed{\text{neutron EDM} = d_n \simeq (\partial d_n / \partial \bar{\theta})|_{\bar{\theta}=0} \times \bar{\theta} \simeq [-0.0050(4)(8)\ e\,\mathrm{fm}] \times \bar{\theta},} \tag{41}$$

  i.e. a nonzero *first derivative at* $\bar{\theta} = 0$, *not* a nonzero EDM at $\bar{\theta} = 0$.
- CP symmetry requires $d_n(0) = 0$, but does *not* require $\partial d_n / \partial \bar{\theta}\big|_0 = 0$.
- Thus their calculation does **not** establish that $\bar{\theta}$ must be an independent physical coupling of QCD.

A nonzero response to a $\bar{\theta}$ source does not establish the physical existence of an independent physical $\bar{\theta}$ coupling.

Hamiltonian formulation: labelling classical vacua

First construct the QCD Hamiltonian. On a spatial slice $\mathbb{R}^3$ of spacetime, impose the *additional* asymptotic condition on the space of allowable smooth *gauge transformations*:,

$$U(\mathbf{x}) \to U_\infty \text{ as } |\mathbf{x}| \to \infty, \text{ i.e., } \textit{assume} \text{ the same limit } U_\infty \text{ in all spatial directions.} \tag{42}$$

Then spatial infinity can be identified to one point,

$$\mathbb{R}^3 \cup \{\infty\} \simeq S^3, \qquad U : S^3 \to SU(3), \qquad \pi_3(SU(3)) = \mathbb{Z}. \tag{43}$$

- All such spatial gauge transformations are labelled by integer winding number n.
- $n = 0$: small gauge transformations – generated locally by Gauss' law.
- $n \neq 0$: large gauge transformations – *not* generated by continuously exponentiating the local Gauss-law constraint.
- Classical vacua have $F_{ij} = 0$ and are pure gauge. Acting on $A_i = 0$ with U_n gives
$$A_i^{(n)} = (i/g) U_n \partial_i U_n^\dagger. \tag{44}$$
Thus the winding classification of U_n induces an integer n labelling of the classical vacuum configurations $A_i^{(n)}$.

The integer classification follows from assuming smoothness and the global asymptotic condition U_∞ at spatial infinity.

Hamiltonian formulation: Chern–Simons number and instantons

At the level of classical fields: The Chern–Simons functional $N_{\rm CS}[A]$ is a functional of the spatial gauge field with the important transformation property

$$\boxed{N_{\rm CS}[A^{U_n}] = N_{\rm CS}[A] + n,} \tag{45}$$

where n is the winding number of the restricted class of gauge transformations, U_n.

- Choosing $N_{\rm CS}[A=0]=0$ then gives for the classical pure-gauge vacua $\boxed{N_{\rm CS}[A^{(n)}] = n}$.
- The 4-dim topological charge density satisfies $q(x) = \partial_\mu K^\mu(x)$, where K^μ is the Chern–Simons current.
- For a sufficiently smooth Euclidean field interpolating between vacuum configurations at $x_4 = -\infty$ and $+\infty$,

$$\boxed{Q = \int d^4x_E\, q_E(x) = N_{\rm CS}(+\infty) - N_{\rm CS}(-\infty).} \tag{46}$$

- Hence a $Q=1$ instanton has the semiclassical interpretation of a transition between neighboring classical vacua, $n \to n+1$.

Instantons provide the Euclidean semiclassical interpolation between the integer-labelled classical vacua of the Hamiltonian picture.

Hamiltonian Formulation: The θ vacuum

After quantization, the local Gauss-law constraint $\hat{G}^a(\mathbf{x})\,|\psi_{\rm phys}\rangle = 0$,

$\Rightarrow$ physical states are invariant under small gauge transformations.

- Gauss' law does *not* determine large gauge transformations U_n on physical states.
- Let $\hat{U}_n$ be the operator versions of the large gauge transformations on physical states. Since winding numbers add, $\hat{U}_m\hat{U}_n = \hat{U}_{m+n}$, and so

$$\Rightarrow \text{ 1-dim unitary representation is } \quad \hat{U}_n\,|\psi\rangle = e^{-in\theta}\,|\psi\rangle \quad \text{for some } \theta \sim \theta + 2\pi. \tag{47}$$

- Physical states must be invariant up to a phase under all gauge transformations, small and large. If $U_1\,|\psi_{\rm phys}\rangle = e^{-i\theta}\,|\psi_{\rm phys}\rangle$ then $U_n\,|\psi_{\rm phys}\rangle = e^{-in\theta}\,|\psi_{\rm phys}\rangle$.
- So the Hilbert space of physical stated can be decomposed as $\mathcal{H}_{\rm phys} = \int^{\oplus} d\theta\,\mathcal{H}_\theta$.
- Now denote the physical states in $\mathcal{H}_\theta$ as $|\psi_\theta\rangle \in \mathcal{H}_\theta$.
- States in different $\mathcal{H}_\theta$ cannot be connected by local gauge-invariant observables $\Rightarrow$ θ superselection sectors.

Define $|\theta\rangle$ as the vacuum state in each θ Hilbert space $\mathcal{H}_\theta$. Then $\boxed{\hat{U}_n\,|\theta\rangle = e^{-in\theta}\,|\theta\rangle}$.

Different values of θ correspond to different realizations of the quantum theory with different Hilbert spaces $\mathcal{H}_\theta$ and different vacua $|\theta\rangle \in \mathcal{H}_\theta$.

Hamiltonian formulation: Semiclassical picture

The preceding θ-sector construction does not require a semiclassical picture. However, it has a useful semiclassical interpretation.

- Recall the classical pure-gauge vacua $A_i^{(n)} = (i/g)U_n \partial_i U_n^\dagger$ with $N_{\rm CS}[A^{(n)}] = n$.
- Semiclassically, associate a state $|n\rangle$ localized about each classical vacuum $A_i^{(n)}$.
- Large gauge transformations shift these states, $\boxed{\hat{U}_m |n\rangle = |n+m\rangle}$.
- Instantons provide the Euclidean semiclassical interpolation between neighboring configurations, $Q = N_{\rm CS}(+\infty) - N_{\rm CS}(-\infty)$ with $Q = \pm 1 \;\Rightarrow\; n \to n \pm 1$.
- The simultaneous eigenstates of all $\hat{U}_m$ are therefore the Fourier superpositions

$$\boxed{|\theta_{\rm semiclass}\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta} |n\rangle \,, \quad \text{so that} \quad \hat{U}_m |\theta_{\rm semiclass}\rangle = e^{-im\theta} |\theta_{\rm semiclass}\rangle \,.} \tag{48}$$

- This is just how $|\theta\rangle$ transforms and so we understand that $\boxed{|\theta\rangle \xrightarrow{\text{semiclassical}} |\theta_{\rm semiclass}\rangle}$.

The familiar "n-vacua + instanton tunneling" picture is a semiclassical realization of the formal Hilbert space θ-sector structure.