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Mixed states from anomalies

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There are several instances where quantum anomalies of continuous and discrete classical symmetries play an important role in fundamental physics. Examples come from chiral anomalies in the Standard Model of fundamental interactions and gravitational anomalies in string theories. Their generic origin is the fact that classical symmetries may not preserve the domains of quantum operators like the Hamiltonian. In this work, we show by simple examples that anomalous symmetries can often be implemented at the expense of working with mixed states having nonzero entropies. In particular there is the result on color breaking by non-abelian magnetic monopoles. This anomaly can be rectified by using impure states. We also argue that non-abelian groups of twisted bundles are always anomalous for pure states sharpening an earlier argument of Sorkin and Balachandran [A. P. Balachandran, G. Marmo, B. S. Skagerstam, and A. Stern, *Classical Topology and Quantum States* (World Scientific, Singapore, 1991).]. This is the case of mapping class groups of geons [A. P. Balachandran, G. Marmo, B. S. Skagerstam, and A. Stern, *Classical Topology and Quantum States* (World Scientific, Singapore, 1991).] indicating that *large* diffeos are anomalous for pure states in the presence of geons. Nevertheless diffeo invariance may be restored by using impure states. This work concludes with examples of these ideas drawn from molecular physics. The above approach using impure states is entirely equivalent to restricting all states to the algebra of observables invariant under the anomalous symmetries. For anomalous gauge groups such as color, this would mean that we work with observables singlet under global gauge transformations. For color, this will mean that we work with color singlets, a reasonable constraint.

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I. INTRODUCTION

There is perhaps a dominant perception that quantum anomalies of classical symmetries can occur only in the context of quantum field theories. Typically they arise in the course of regularizing divergent expressions in quantum fields [1,2], causing the impression that it is these divergences that cause anomalies.

It is however known that anomalies can occur in simple quantum mechanical systems such as a particle on a circle or a rigid rotor. Esteve [3,4] explained long ago that the presence or otherwise of anomalies is a problem of domains of quantum operators. Thus while quantum state vectors span a Hilbert space $\mathcal{H}$, the Hamiltonian H is seldom defined on all vectors of $\mathcal{H}$. For example, the space $\mathcal{H}$ of square-integrable functions on R^3 contains nondifferentiable functions ψ, but the Schroedinger Hamiltonian $H = -\frac{1}{2m}\nabla^2$ is not defined on such ψ. Rather H is defined only on a dense subspace D_H of $\mathcal{H}$. If a classical symmetry g does not preserve D_H, $gD_H \neq D_H$, then $Hg\psi$ for $\psi \in D_H$ is an ill-defined expression. In this case, one says that g is anomalous [3,4]. See also [5–11].

In the present work, we explore the possibility of overcoming anomalies by using mixed states. There are excellent reasons for trying to do so, there being classical gauge symmetries like $SU(3)$ of QCD or *large* diffeomorphisms (diffeos) of manifolds (see below) which can become anomalous. Color $SU(3)$ does so in the presence of non-abelian monopoles [12–14], while "large" diffeos do so for suitable Friedman-Sorkin geon manifolds [15–17]. It is surely worthwhile to find ways to properly implement these symmetries.

In this paper, we first focus on simple quantum mechanical systems to illustrate how the use of impure states can often restore the anomalous symmetries. We then discuss color breaking by non-abelian monopoles. Finally we argue that structure groups of twisted non-abelian bundles are *always* anomalous for pure states. This claim is illustrated with examples from molecular physics, where such groups are not only compact, but discrete as well. In later work, we will extend these considerations to diffeo anomalies.

While non-abelian structure groups of twisted bundles are always anomalous, abelian groups also of course can be

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anomalous. For instance, parity anomaly for a particle on a circle (discussed in Sec. II of this work) and the axial $U(1)_A$ anomaly in the Standard Model are both abelian. The crucial issue is whether the classical symmetry preserves the domains of appropriate operators like the Hamiltonian. If they do not preserve such domains, then they are anomalous. The important feature of non-abelian structure groups of twisted bundles is that they *never* preserve the domain of the Hamiltonian. More on this later.

Our use of mixed states is entirely equivalent to restricting the algebra of observables to those invariant under symmetries. For global symmetries, this can be a restriction, as there may be no good reason to discard noninvariant observables. But for many *gauge* symmetries, this requirement is often already implied by gauge invariance. That is the case for mapping class groups of manifolds and "symmetries" of molecules. For the global color group which is emergent from gauge transformations, constraining observables to singlets is reasonable in view of the hypothesis of color confinement.

In this paper, all examples we work on are those of global anomalies. As a matter of specificity, most of these examples are of "global" gauge anomalies like the global color group or large diffeos.

We shall see that even though we can overcome the problem of implementing a symmetry, time evolution still does involve the choice of a domain. In this sense, the theory carries the memory of the anomaly.

But when the anomaly is for a classical symmetry, a domain and its transform by this symmetry are *equivalent*, exactly as in the case of standard spontaneous symmetry breaking. In quantum field theory, there seems to be an associated Nambu-Goldstone theorem as well. But now we can show that all this can happen on a spatial manifold with a boundary, and does not require its infinite volume. We will elaborate on these issues elsewhere.

The present paper is organized as follows: in Sec. II, we discuss parity and time reversal for a particle on a circle, this being a very simple example; In Sec. III, we adapt this discussion to color breaking; In Sec. IV, we show the generic nature of our results. We finally conclude with examples from molecular physics.

II. ANOMALOUS PARITY AND TIME REVERSAL FOR PARTICLE ON A CIRCLE

A. Classical theory

A point on a circle S^1 can be described by $e^{i\varphi}$, with φ being real. Its classical equation of motion assuming it to be free is

$$\frac{d^2}{dt^2}\varphi(t) = 0, \tag{1}$$

where t labels time.

If S^1 is embedded in R^2,

$$S^1 = \{x = (x_1, x_2) \in \mathsf{R}^2\colon x_1^2 + x_2^2 = 1\}, \tag{2}$$

then we can relate $e^{i\varphi}$ to x by writing

$$x_1 + ix_2 = e^{i\varphi}. \tag{3}$$

The parity transformation $P\colon (x_1, x_2) \mapsto (x_1, -x_2)$ takes $e^{i\varphi}$ to $e^{-i\varphi}$, that is,

$$P\colon e^{i\varphi} \mapsto e^{-i\varphi}. \tag{4}$$

It is an orientation-reversing diffeomorphism of S^1. On the angular variable $\varphi \in [0, 2\pi]$, its action is $P\colon \varphi \mapsto 2\pi - \varphi$. Classically (4) is a symmetry of the equation of motion (1).

The time-reversal transformation T defined by

$$T\colon e^{i\varphi(t)} \mapsto e^{-i\varphi(-t)} \tag{5}$$

is also a classical symmetry.

B. Quantum theory

In quantum theory, the Hamiltonian H from which one can obtain (1) is

$$H = -\frac{1}{R}\frac{d^2}{d\varphi^2}, \tag{6}$$

where the constant $1/R$ has the dimension of energy.

The Hilbert space for a particle on S^1 is

$$\mathcal{H} \equiv L^2(S^1) = \{\langle \chi, \psi\rangle := \int_0^{2\pi} d\varphi\, \bar{\chi}\psi < \infty, \quad \text{for } \chi, \psi \in L^2(S^1)\}. \tag{7}$$

As usual, $\langle \psi, \psi\rangle = \|\psi\|^2$.

Now, the Hamiltonian H has several different domains for which it is self-adjoint. They are labeled by the points $\eta = e^{i\theta}$ of S^1. The definition of these domains is[1]

$$D_\eta = \{\psi \in \mathcal{H}\colon \psi(2\pi) = \eta\psi(0)\}. \tag{8}$$

The density matrix $|\psi\rangle\langle\psi|$ associated to $\psi \in D_\eta$ is a periodic function of φ, since η cancels out, showing that (6) is appropriate for quantum dynamics on S^1.

Another way to see that (8) is good for quantum dynamics on S^1 is the following. Let us consider the algebra $\mathsf{C}^\infty(S^1)$ of smooth functions on S^1. Then D_η is a module for $\mathsf{C}^\infty(S^1)$, that is, if $f \in \mathsf{C}^\infty(S^1)$ and $\psi \in D_\eta$, then

$$f\psi \in D_\eta. \tag{9}$$

As S^1 can be recovered from $\mathsf{C}^\infty(S^1)$ as a topological space by the Gel'fand-Naimark theorem[2] [18], we again see that (8) works out.

[1]There are also some differentiability (Sobolev) conditions for ψ in these domains.

[2]The closure of $\mathsf{C}^\infty(S^1)$ in the sup-norm gives a C^*-algebra to which we can apply the Gel'fand-Naimark theorem.

All of these remarks go towards solving an old problem of the *Quantum Baby* described in detail in [19].

1. Parity

Parity P acts on ψ according to

$$(P\psi)(\varphi) = \psi(2\pi - \varphi). \quad (10)$$

Hence, if $\psi \in D_\eta$, then

$$(P\psi)(2\pi) = \psi(0) = \bar{\eta}\psi(2\pi) = \bar{\eta}(P\psi)(0), \quad (11)$$

or $P\psi \in D_{\bar{\eta}}$, that is,

$$PD_\eta = D_{\bar{\eta}}. \quad (12)$$

The conclusion is that P is anomalous unless $\eta = \bar{\eta}$ or $\eta = \pm 1$. In terms of θ, the statement is that P is anomalous unless $\theta = 0, \pi \bmod 2\pi$.

2. Time reversal

Since T is an anti-unitary operator,

$$TD_\eta = D_{\bar{\eta}}, \quad (13)$$

so T as well is broken, unless again $\eta = \bar{\eta}$ or $\eta = \pm 1$.

Note however that PT preserves D_η for all η,

$$PTD_\eta = D_\eta. \quad (14)$$

Recall that in $1 + 1$ QED and $3 + 1$ QCD, the well-known θ-terms also break P and T, unless $\theta = 0, \pi$, while PT is always preserved. This coincidence is not accidental. It comes from the fact that $\pi_1(Q) = \mathbb{Z}$ for their configuration spaces Q [20,35].

3. Restoration of P and T

A naive approach to restoration of P and T, which however does not work, is the following. Consider the case of P. For $\psi, \chi \in D_\eta$, we can declare that the domain of H consists of vectors of the form $\psi + P\chi$. Since ψ or χ can be zero, this means that we would like to declare the linear span D of D_η and PD_η as the domain of H.

This approach does not work as D is not a domain for H. An easy way to see this fact is to check that

$$\langle \psi + P\chi, H(\psi + P\chi)\rangle - \langle H(\psi + P\chi), \psi + P\chi\rangle \quad (15)$$

is not zero for generic ψ, χ. So H is not even symmetric on D.

Another, but different, reason to discard such D is to note that

$$|\psi + P\chi\rangle\langle\psi + P\chi| \quad (16)$$

is not a periodic function of S^1 for generic ψ, χ. Thus D is not adapted to the quantum particle problem on S^1.

Now, if we do not insist that H is always defined, but only the unitary time evolution e^{-itH} is, then as this is a bounded operator, it is defined on all of $\mathcal{H}$, an hence also on D. For this definition of e^{-itH}, we can start with H having domain D_η, and define e^{-itH} on D_η and then extend it to all of $\mathcal{H}$ (see below). However this will not resolve the second difficulty noted above, as D is still not adapted to an underlying S^1. Furthermore, the evolutions e^{-itH} are different if the starting domain is D_η or $D_{\bar{\eta}}$ (if $\eta \neq \bar{\eta}$), for instance.

Thus such superpositions of vectors to overcome anomalies in P or T do not work.

There is an alternative though. For $\psi \in D_\eta$, we note that

$$\Omega = |\psi\rangle\langle\psi| + P|\psi\rangle\langle\psi|P \quad (17)$$

has positive trace if $|\psi\rangle$ is not a zero vector, that is,

$$\mathrm{Tr}\,\Omega = 2\langle\psi, \psi\rangle > 0. \quad (18)$$

Hence

$$\omega = \frac{\Omega}{\Omega}, \qquad \mathrm{Tr}\omega = 1, \quad (19)$$

is a well-defined state on observables. Moreover it is P and T invariant and is continuous on S^1.

If $K = K^\dagger$ is a (bounded) observable, its mean value in this state is defined by

$$\omega(K) = \mathrm{Tr}K\omega = \frac{1}{\mathrm{Tr}\Omega}[\langle\psi|K|\psi\rangle + \langle\psi|PKP|\psi\rangle]. \quad (20)$$

Since

$$\omega(K) = \omega(PKP), \quad (21)$$

then $\omega(K)$ is zero for P-odd K:

$$\omega(K) = 0, \quad \text{if } PKP = -K. \quad (22)$$

If P were not anomalous, so that $\eta = \pm 1$, then $\psi \in D_\eta$ need not be an eigenstate of P. So $|\psi\rangle\langle\psi|$ may have no definite parity, and P-odd observables K may have non-trivial expectation values $\langle\psi|K|\psi\rangle$.

As for time evolution, it is important to keep its group property. So we can time-evolve $|\psi\rangle$ by e^{-itH_η} or $e^{-itH_{\bar{\eta}}}$ to obtain $|\psi_t\rangle_\eta$ or $|\psi_t\rangle_{\bar{\eta}}$. We can then use (20) to calculate the mean value of K. As this mean value does depend on η, we still have two physically distinct choices for time evolution.

Note that P-invariant observables form a subalgebra.

Our rule (20) for expectation values can actually be derived by restricting ω to P-invariant operators. Thus if PKP is K, then

$$\langle\psi|PKP|\psi\rangle = \langle\psi|K|\psi\rangle = \frac{1}{2}[\langle\psi|PKP|\psi\rangle + \langle\psi|K|\psi\rangle], \quad (23)$$

which leads to (20). We have emphasized the significance of this result for gauge theories in the introduction.

All the above remarks are seen to straightforwardly apply to time reversal T.

4. Summary

In the presence of P and T anomalies, we can restore them compatibly with time evolution. We must however work with *impure states* ω of rank 2. We must work with P-invariant states and so also P-invariant observables.

For anomalous *gauge* symmetries like color, this is actually good, as it gives the possibility of restoring gauge invariance.

C. What is an anomaly?

In the general formulation of quantum theory, it is assumed that any bounded self-adjoint operator K is an observable. Being bounded, it is defined on all of $\mathcal{H}$. Such K can however mix domains.

Let us consider, for example, the unitary operator $U_{\eta'}$, with $\eta' = e^{i\theta'}$, defined by

$$(U_{\eta'}\psi)(\varphi) = e^{i(\theta'/2\pi)\varphi}\psi(\varphi). \tag{24}$$

Acting with this operator on D_η, one changes η to $\eta'\eta$, i.e.,

$$U_{\eta'}D_\eta = D_{\eta'\eta}. \tag{25}$$

Moreover, since $U_{\eta'}$ is a bounded operator, it is defined on all of $\mathcal{H}$.

Now, the operators

$$K = \frac{1}{2}(U_{\eta'} + U^\dagger_{\eta'}), \tag{26}$$

$$K' = \frac{1}{2i}(U_{\eta'} - U^\dagger_{\eta'}) \tag{27}$$

are bounded and self-adjoint. Are they observables?

In fact, the parity operator P is bounded and self-adjoint. Is it an observable? If yes, is its anomaly problem spurious?

A closer examination reveals that in the presence of domain-changing observables, there is no canonical choice for time evolution. Any choice will fail to commute with the domain-changing observable. We have already remarked on this point and its relation to spontaneous symmetry breaking. That is so even if it generates a classical symmetry like P. In the latter case, we call the classical symmetry anomalous.

Extension of e^{-itH_η} to all of $\mathcal{H}$

We begin by solving the eigenvalue problem

$$H_\eta\psi^\eta_n = E_n\psi^\eta_n. \tag{28}$$

The solution is (recalling that $\eta = e^{i\theta}$ and $\psi^\eta_n \in D_\eta$)

$$\psi^\eta_n(\varphi) = \frac{1}{\sqrt{2\pi}}e^{i(n+(\theta/2\pi))}\varphi, \tag{29}$$

$$E_n = \frac{1}{R}\left(n + \frac{\theta}{2\pi}\right)^2, \quad \text{with} \quad n \in \mathbb{Z}. \tag{30}$$

Now, $\{\psi^\eta_n\}$ is a complete set. So any $\chi \in \mathcal{H}$, even if it is not in D_η, can be expanded in the basis $\{\psi^\eta_n\}$:

$$\chi = \sum_n a_n\psi^\eta_n \tag{31}$$

$$a_n = (\psi^\eta_n, \chi). \tag{32}$$

The expansion converges in norm, that is,

$$\lim_{N\to\infty}\|\chi - \sum_{|n|\le N}a_n\psi^\eta_n\| = 0. \tag{33}$$

The time evolution of χ under e^{-itH_η} is

$$\chi_t = e^{-itH_\eta}\chi_0 = \sum_{|n|\le N}a_n e^{-itE_n}\psi^\eta_n, \tag{34}$$

for a initial $\chi_0 = \chi$. The R.H.S. converges, since $|a_n e^{-itE_n}| = |a_n|$.

But if $\chi_t D_\eta$, term-by-term differentiation of the R.H.S. in t leads to a divergent series.

We can illustrate this by considering a periodic χ and $\eta \neq 1$. Set

$$\chi(\varphi) = \chi_M(\varphi) = \frac{1}{2\pi}e^{iM\varphi}, \qquad M \in \mathbb{Z}. \tag{35}$$

Then

$$\begin{aligned} a_n &= \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i(n+(\theta/2\pi))\varphi}e^{iM\varphi} \\ &= \frac{1}{2\pi}\frac{i}{n + \frac{\theta}{2\pi} - M}(e^{-i\theta} - 1). \end{aligned} \tag{36}$$

With these a_n, the series (31) and (34) converge since $|a_n| = O(\frac{1}{n^2})$ as $|n| \to \infty$:

$$\sum_n |a_n|^2 < \infty. \tag{37}$$

But term-by-term differentiation of (31) leads to a divergent series since $|a_n E_n| = O(|n|)$ as $n \to \infty$.

The conclusion is that time evolution $U_\eta(t)$ determined by H_η is defined on all $\mathcal{H}$ (and is continuous in t), but is differentiable in t only on vectors in the domain D_η of the Hamiltonian H_η. If a classical symmetry g does not preserve this domain, then $gU_\eta(t) - U_\eta(t)g \neq 0$ on all of $\mathcal{H}$, and we say that g is anomalous.

D. Relation to Lagrangian approach

In this subsection, we explain how our discussion of anomalies based on domains can be interpreted in conventional terms. The example of the particle on a circle gives a transparent model for this demonstration.

Consider the operator

$$U_{\bar{\eta}}\colon (U_{\bar{\eta}}\psi)(\varphi) = e^{-i(\theta/2\pi)\varphi}\psi(\varphi). \tag{38}$$

For $\psi \in D_\eta$, then

$$U_{\bar{\eta}}\psi \in D_1. \tag{39}$$

Now, D_1 consists of periodic functions and it is invariant under parity. But the new Hamiltonian

$$H_\eta = U_{\bar{\eta}} H U_{\bar{\eta}}^{-1} = \frac{1}{R}\left(-i\frac{\partial}{\partial\varphi} + \frac{\theta}{2\pi}\right)^2 \tag{40}$$

is not parity invariant.

Using canonical methods, it is easy to show that the Hamiltonian H_η comes from a Lagrangian

$$L_\eta = \frac{R}{2}\dot{\varphi}^2 - \frac{\theta}{2\pi}\dot{\varphi}. \tag{41}$$

In $L_\eta dt$, $-(\theta/2\pi)d\varphi$ is a topological term. It is closed, but not exact on S^1. It is the analogue of the Wess-Zumino-Witten term [20] or the topological term in the charge-monopole Lagrangian [21].

We can also model "covariant" and "consistent" anomalies of quantum field theory in this model. For this purpose, for clarity, we write $-i(\theta/2\pi)d\varphi$ as a connection:

$$A(\varphi) = e^{i(\theta/2\pi)\varphi} d(e^{-i(\theta/2\pi)\varphi}), \tag{42}$$

so that

$$L_\eta dt = \frac{R}{2}\dot{\varphi}^2 dt - iA(\varphi) \tag{43}$$

Note that we can allow any fluctuation in A, which is an exact one-form on S^1 without affecting the cohomology class of A. Such fluctuations will not change the domain D_η of the Hamiltonian. Let us allow such fluctuations now.

For that we write

$$A = -ia(\varphi)d\varphi \tag{44}$$

and

$$L_\eta = \frac{R}{2}\dot{\varphi}^2 - a(\varphi)\dot{\varphi}. \tag{45}$$

This Lagrangian defines a model invariant under the "small" gauge transformations

$$a(\varphi) \to a(\varphi) + \frac{\partial\Lambda}{\partial\varphi}, \tag{46}$$

$$\Lambda(2\pi) = \Lambda(0) \bmod 2\pi, \tag{47}$$

as they change (45) only by a total derivative $-d\Lambda/dt$. Furthermore, it preserves the domain D_η. Hence they preserve the spectrum of the Hamiltonian. [The meaning of the mod 2π qualification in (47) is that $e^{i\Lambda(\varphi)}$ defines a $U(1)$-valued function on S^1.]

If a Maxwell term $F^2(\phi)$ is introduced for $a(\phi)$, the Gauss law reads

$$\frac{\partial E(\phi)}{\partial\phi} - \frac{\theta}{2\pi}\delta(\phi - \varphi) = 0, \tag{48}$$

where $E(\phi)$ is the electric field. This is the analogue of the Gauss law in the presence of a point charge at $z(t)$ at time t:

$$\frac{\partial E^i(x)}{\partial x^i} + e\delta^3(x - z(t)) = 0. \tag{49}$$

The charge Q on S^1 is thus given by integrating (48), so that

$$Q = E(2\pi) - E(0) = \frac{\theta}{2\pi}. \tag{50}$$

This charge is conserved. But under an anomalous gauge transformation, where the gauge function Λ does not fulfill (47), θ changes. So it is not invariant under such gauge transformations. It is thus the analogue of the consistent charge. The corresponding consistent but not gauge invariant current

$$\frac{\partial E(\phi)}{\partial\phi} - \frac{\theta}{2\pi}\delta(\phi - \varphi) \tag{51}$$

happens to be zero here. The corresponding covariant gauge invariant current is

$$\frac{\partial E(\phi)}{\partial\phi}. \tag{52}$$

III. NON-ABELIAN MONOPOLES AND BREAKDOWN OF COLOR

In 't Hooft-Polyakov models, magnetic monopoles are associated with twisted G-bundles on the sphere S^2_∞ at ∞. Here, G is the remaining gauge symmetry group after the breaking $G^{(0)} \to G$ by a Higgs field Φ. This remaining group G is also known as global or large gauge group. Furthermore, S^2_∞ refers to a large enough spatial sphere, where Φ can be approximated by its asymptotic value Φ_∞.

In the unitary gauge, where Φ_∞ takes a constant value on S^2_∞, the G-bundle is described by a transition function on a small strip $\theta \in [\pi/2 - \epsilon, \pi/2 + \epsilon]$ around the equator of S^2_∞, where θ is the polar angle. This is called a *collar neighborhood* N_ϵ of the equator in S^2_∞. When θ lies in N_ϵ and the azimuthal angle φ increases from 0 to 2π, the transition function τ maps this curve to a noncontractible loop in G.

It can happen that the values $\tau(\theta, \varphi)$ taken by τ are not in the center $\mathcal{C}$ of G. In that case $g\tau(\theta, \varphi)g^{-1} \neq \tau(\theta, \varphi)$ for all $g \in G$. The group G is then broken.

As examples, consider $U(2)$ and $U(3)$. The second group contains the color group $SU(3)$ and the electromagnetic $U(1)$, since $U(3) = [SU(3) \times U(1)]/\mathbb{Z}_3$.

Let us first consider $U(2) = (SU(2) \times U(1))/\mathsf{Z}_2$. We work in its two-dimensional (faithful) representation by unitary matrices. Then the choice

$$\tau(\theta, \varphi) = e^{(i/2)\sigma_3\varphi} e^{(i/2)\varphi}, \tag{53}$$

where σ_3 is the third Pauli matrix, gives a noncontractible loop in $U(2)$, which is not entirely contained in its center $U(1)$. The homotopy class of this loop generates $\pi_1[U(2)] = \mathsf{Z}$.

A similar discussion applies to $U(3) = [SU(3) \times U(1)]/\mathsf{Z}_3$. In its three-dimensional irreducible representation, the diagonal matrix $Y = \frac{1}{3}(1, 1, -2)$ is in the Lie algebra $u(3)$ of $U(3)$. The transition function τ defined by

$$\tau(\theta, \varphi) = e^{iY\varphi} e^{-i(2\pi/3)\varphi} \tag{54}$$

is a noncontractible loop which is not contained in the center of $U(3)$. So, for a generic $g \in U(3)$,

$$g\tau(\theta, \varphi)g^{-1} \neq \tau(\theta, \varphi) \tag{55}$$

in the entire collar neighborhood around the equator. Thus, global $SU(3)$ color cannot be implemented.

In [20,35], it was shown that each such τ characterizes a domain D_τ of say the Dirac Hamiltonian H^D. Moreover, global $SU(3)$ color becomes anomalous because its action changes D_τ to $D_{g\tau g^{-1}}$.

We can now restore color as a symmetry by following the procedure described in the last section. Let $|\chi\rangle_\tau$ be a state vector for the transition function τ. This defines its gauge. It is in the domain D_τ.

Suppose a $g \in G$, it acts on τ by conjugation

$$(g\tau g^{-1})(\theta, \varphi) = g\tau(\theta, \varphi)g^{-1}. \tag{56}$$

So

$$gD_\tau = D_{g\tau g^{-1}}. \tag{57}$$

Following Sec. II, we thus consider

$$\Omega = \int_G d\mu(g) g|\chi\rangle_{\tau\tau}\langle\chi|g^\dagger = \int_G d\mu(g)|\chi\rangle_{g\tau g^{-1} g\tau g^{-1}}\langle\chi|, \tag{58}$$

where $d\mu(g)$ is the Haar measure on G.

This Ω is a positive G-invariant operator, so that

$$\omega = \frac{\Omega}{\mathrm{Tr}\,\Omega} \tag{59}$$

is a G-invariant state.

Let H_τ be the Hamiltonian with domain D_τ. On the intersection

$$\bigcap_{g\tau g^{-1}, g\in G} D_{g\tau g^{-1}} = D^0 \tag{60}$$

of these domains, the Hamiltonian $H_{g\tau g^{-1}}$ coincide

$$H_{g\tau g^{-1}}|_{D^0} = H_\tau, \tag{61}$$

for all $g \in G$. Also,

$$g e^{-itH_\tau} g^{-1} = e^{-itH_{g\tau g^{-1}}}. \tag{62}$$

We now define Ω_t at time t by

$$\Omega_t = \int_G d\mu(g) e^{-itH_{g\tau g^{-1}}}|\chi\rangle_{g\tau g^{-1} g\tau g^{-1}}\langle\chi|e^{itH_{g\tau g^{-1}}}, \tag{63}$$

with Ω_0 being Ω. Now, Ω_t is positive and G-invariant. It gives the G-invariant state

$$\omega_t = \frac{\Omega_t}{\Omega_t}. \tag{64}$$

The state ω_t is impure.

Is color confinement a domain problem?

Suppose that there is no twisted $SU(3)$- or more generally twisted G-bundle on spatial slices, so that state vectors $|\chi\rangle$, which are color ($G-$) non-singlets are in the domain of the Hamiltonian. Suppose though that there is "confinement" in the sense that we observe only $SU(3)$-invariant operators K. Such (bounded) operators form an algebra $\mathcal{A}$. Then $|\chi\rangle\langle\chi|$ (with $\langle\chi|\chi\rangle = 1$) restricted to $\mathcal{A}$ is in fact an impure state like the one we discussed before. That is because we can trace over $|\psi\rangle\langle\psi|$ the color degrees of freedom. This point was emphasized by Akant *et al* [22].

To see this explicitly, let $U(g)$ be the unitary operator implementing G. Then for $K \in \mathcal{A}$,

$$\langle\chi|K|\chi\rangle = \frac{1}{V}\int_G d\mu(g)\langle\chi|U(g)^\dagger K U(g)|\chi\rangle, \tag{65}$$

$$V = \int_G d\mu(g), \tag{66}$$

or

$$\mathrm{Tr}\, K|\chi\rangle\langle\chi| = \mathrm{Tr} K\omega, \tag{67}$$

$$\omega = \frac{1}{V} d\mu(g) U(g)|\chi\rangle\langle\chi|U(g)^\dagger. \tag{68}$$

Since the Hamiltonian H must be a G-singlet if H is to display confinement, we can evolve ω for time t in a conventional way,

$$\omega_t = e^{-itH}\omega_0 e^{itH}, \tag{69}$$

with $\omega_0 = \omega$. The previous formula (64) reduces to (69) when there is no domain problem.

However, we were led to the singlet states ω_t of (64) because of domain problems caused by non-abelian monopoles. Is this a first step towards a proof of confinement?

Discussions of confinement also speculate that colored states have infinite mean energy. That is also the case here if this conjecture is suitably interpreted. Thus, first consider e^{-itH_τ}, H_τ being the Hamiltonian with domain D_τ. It can be defined on all $\mathcal{H}$ including vectors $|\chi\rangle_{g\tau g^{-1}}$, with $g\tau g^{-1} \in D_{g\tau g^{-1}} \neq D_\tau$. But

$$i\frac{d}{dt}\langle\chi|e^{-itH_\tau}|\chi\rangle_{g\tau g^{-1}}|_{t=0}g\tau g^{-1} \quad (70)$$

diverges.

We can show this by the parity example of section 2, but the result seems to be generic. Thus from (28), (29), (31), and (36), and also

$$\langle\chi_M|e^{-itH_\eta}|\chi_M\rangle = \sum_n |a_n|^2 e^{-itE_n}, \quad (71)$$

it follows that

$$E_n = \frac{1}{R}\left(n + \frac{\theta}{2\pi}\right)^2 \quad (72)$$

$$a_n = \frac{1}{2\pi}\frac{1}{n + \frac{\theta}{2\pi} - M}(e^{-i\theta} - 1), \quad (73)$$

showing that (71) is not differentiable in t or that the mean energy $\langle\chi_M|H_\eta|\chi_M\rangle$ is infinite.

This is perhaps a mechanism which contributes to confinement. But for further progress, we still need nonabelian colored monopoles associated with reasonable length scales. Unfortunately, we know of none. GUT monopoles seem too small for our purpose. If the length scale of quark confinement is 10^{28} cm^{-1}, then it is hard to understand the low-energy success of the quark model.

IV. ON THE GENERICITY OF GAUGE ANOMALIES

Let $\hat{G}$ be a gauge group for a quantum system based on a Hamiltonian H. *By definition*, all observables, including H, commute classically with $\hat{G}$.

In quantum theory, typically, the identity component $\hat{G}_0$ of $\hat{G}$ is required to act trivially on quantum states by virtue of a Gauss law. The group $\hat{G}/\hat{G}_0 = G$ can then act by an unitary irreducible representation (UIRR) ρ on the quantum states.

As an example, consider QCD. There, for $\hat{G}$, we can consider $\mathcal{G}^\infty(SU(3))$, the group of maps from $\mathbb{R}^3$ to $SU(3)$, which reduce to identity at spatial infinity. Its identity component $\mathcal{G}_0^\infty(SU(3))$, being generated by Gauss law, acts trivially on quantum states. Now, $\mathcal{G}^\infty(SU(3))/\mathcal{G}_0^\infty(SU(3)) = \pi_3(SU(3)) = \mathbb{Z}$. It has UIRR's $\rho \equiv \rho_\theta$ with $\rho_\theta(n) = e^{in\theta}$ for $n \in \mathbb{Z}$. The angle θ is fixed in a given QCD theory.

In quantum gravity based on asymptotically flat spacetimes, the approach of diffeomorphisms $D^\infty(M)$ of the spatial slice M which become asymptotically identity plays a role similar to $\mathcal{G}^\infty(SU(3))$. Its identity component $D_0^\infty(M)$ acts trivially on quantum states, while the discrete group $D^\infty(M)/D_0^\infty(M)$ acts by some UIRR ρ on quantum states.

There are examples of a different sort from molecular physics [20]. In the Born-Oppenheimer approximation, the family of nuclear orientations which serves as the configuration space Q for rotational excitations is $SU(2)/G$, where G is a subgroup of $SU(2)$. It may be discrete giving rise to a Platonic solid [23], $U(1)$ or $\mathbb{Z}_4 \ltimes U(1)$. If $U(1) = \{e^{i\theta\sigma_3/2}, 0 \leq \theta \leq 4\pi\}$ and $\mathbb{Z}_4 = \{z = i\sigma_2 : z^4 = e\}$, then it is generated by $\langle e^{i\theta\sigma_3/2}, i\sigma_2\rangle$.

In time-reversal invariant systems, if the value $\mathbf{k}_0$ of momentum $\mathbf{k}$ is time-reversal invariant, then the sphere $\{\mathbf{k}: |\mathbf{k} - \mathbf{k}_0|^2 = 1\}$ can support a $\mathbb{Z}_2$-bundle [12–14,24]. The $\mathbb{Z}_2$ is generated by the square of the time-reversal transformation T. According to Wigner [25], T^2 is either $+1$ or -1. T can act on quantum states by either of these two UIRR's. Since observables necessarily commute with the square of time-reversal transformation, $\mathbb{Z}_2$ is a gauge group. These bundles occur in discussions of topological insulators [26].

Thus there are plenty of gauge groups G and many are non-abelian.

Let us call the effective gauge group after possible Gauss-law constraints are accounted for as G. As explained above, it is the group which can act by nontrivial representations ρ on quantum states.

Now if $\rho(g)$ is the unitary operator representing $g \in G$ on quantum states, then ρ also gives a representation of the entire group algebra $\mathbb{C}G$ of G. If $\sum_g c(g)g \in \mathbb{C}G$, where $c(g) \in \mathbb{C}$, then its operator is $\sum_g c(g)\rho(g)$. This representation incidentally is a *-representation:

$$*: \sum_g c(g)g \rightarrow \sum_g \bar{c(g)}\, g^{-1} \quad (74)$$

on $\mathbb{C}G$ goes over to the adjoint operations in the representation

$$\rho\left(\sum_g \bar{c(g)}\, g^{-1}\right) = \left(\sum_g c(g)\rho(g)\right)^\dagger, \quad (75)$$

since $\rho(g)^\dagger = \rho(g^{-1})$.

Now all observables must commute with $\mathbb{C}\hat{G}$, the gauge group algebra of $\hat{G}$, and, in particular, with $\mathbb{C}G$. That is the meaning of gauge invariance. But if G and hence $\mathbb{C}G$ are non-abelian, only the center $\mathcal{C}(\mathbb{C}G)$ of $\mathbb{C}G$ commutes with every element of $\mathbb{C}G$. If G is abelian, the $\mathcal{C}(\mathbb{C}G) = \mathbb{C}G$, but that is not the case if G is non-abelian.

Thus if G is a finite group, its center has the basis [27]

$$e_\alpha = \sum_g \chi_\alpha(g)g, \quad (76)$$

where χ_α is the character in the irreducible representation ρ_α. If instead G is a compact Lie group, its center is spanned by the Casimir invariants. In either of these cases of interest, $\mathcal{C}(\mathbb{C}G)$ is an *abelian* algebra.

Since $\mathcal{C}(\mathbb{C}G)$ lies in the center of the entire algebra of observables, in a given representation of the latter, elements of $\mathcal{C}(\mathbb{C}G)$ have a fixed value. Fixing e_α means fixing the irreducible representation[3] while for Lie groups G, we will be fixing its Casimirs.

Thus, general considerations fix *only* the UIRR ρ of $\mathbb{C}G$. The $\rho(g)$ acts on a Hilbert space $\mathcal{H}$ by a unitary representation, so we can choose a complete set spanning $\mathcal{H}$ in the form

$$|\sigma\rangle \otimes |\psi\rangle \equiv |\sigma, \psi\rangle, \tag{77}$$

where

$$\rho(g)|\sigma, \psi\rangle = |\sigma', \psi\rangle \rho(g)_{\sigma'\sigma}, \tag{78}$$

on denoting the matrix of $\rho(g)$ by the same symbol.

Now, elements of $\rho(\mathcal{C}(\mathbb{C}G))$ have exactly the same value on $|\sigma, \psi\rangle$, for every $\sigma \in \mathcal{C}(\mathbb{C}G)$, with ρ being irreducible. So $\mathcal{C}(\mathbb{C}G)$ does not mix different values of σ, nor does any other observable as it commutes with $\rho(G)$. So we have to "gauge fix" the redundancy in the multiplicity of of σ if possible.

We are assuming that the dimension of $\rho(G)$ is larger than one, otherwise $\rho(\mathbb{C}G)$ is abelian.

One possibility that may occur is that we can fix the value for σ, and choose a domain for observables in the span of $\{|\psi\rangle\}$. This may be possible with observables acting just on $|\psi\rangle$. The ψ's are typically functions on a classical configuration space Q, so that in this case the quantum vector bundle over Q is trivial. Physical predictions in this case do not depend on σ.

Instead of working with vector states, we can also work with density matrices

$$\sum_\sigma \frac{|\sigma, \psi\rangle\langle\sigma, \psi|}{\mathrm{Tr}|\sigma, \psi\rangle\langle\sigma, \psi|}. \tag{79}$$

Such states are more like our construction in Sec. II and treat all σ democratically. However, on observables, both approaches are equivalent when the bundle is trivial.

Note also that G acts on (79) by the identity representation,[4] while if we gauge fix σ, the G-action changes the gauge, but harmlessly.

When the bundle is twisted, we cannot proceed in this manner. In that case, we cover Q by contractible open sets Q_α,

$$Q = \bigcup_\alpha Q_\alpha. \tag{80}$$

In each Q_α, we choose a section

$$\sum_\sigma \chi_\sigma^{(\alpha)}|\sigma, \psi\rangle, \tag{81}$$

where $\chi_\sigma^{(\alpha)}$ are smooth functions on Q_α. In the overlap $Q_{\alpha\beta} = Q_\alpha \cap Q_\beta$, we have a transition function $U_{\alpha\beta}$, which at $q \in Q_{\alpha\beta}$ gives an element $\rho(g)$, $g \in G$,

$$U_{\alpha\beta} \in \rho(G), \qquad q \in Q_{\alpha\beta}, \tag{82}$$

in a self-evident notation. Then the vectors (81) and

$$\sum_\sigma \chi_\sigma^{(\beta)}|\sigma, \psi\rangle \tag{83}$$

are related by $U_{\alpha\beta}$ over $Q_{\alpha\beta}$:

$$\sum_\sigma \chi_\sigma^{(\alpha)}|\sigma, \psi\rangle = U_{\alpha\beta}\sum_\sigma \chi_\sigma^{(\beta)}|\sigma, \psi\rangle \quad \text{on } Q_{\alpha\beta}. \tag{84}$$

There are also consistency conditions on $U_{\alpha\beta}$ which lead to Čech cohomology [28,29].

If there exist U_α's which are $\rho(G)$-valued smooth functions on Q_α such that

$$U_{\alpha\beta} = U_\alpha^{-1}U_\beta \quad \text{on } Q_{\alpha\beta}, \tag{85}$$

then we can reduce $U_{\alpha\beta}$ to the constant function on $Q_{\alpha\beta}$ with value 1 by choosing different sections, namely

$$U_\alpha \sum_\sigma \chi_\sigma^{(\alpha)}|\sigma, \psi\rangle \quad \text{on } Q_\alpha. \tag{86}$$

But such U_α may not exist. In that case, the vector bundle is said to be "twisted."

The choice of sections on Q_α is a "gauge choice." It also goes towards fixing the domain of the Hamiltonian.

If the vector bundle is twisted, we cannot say that the action of $\rho(g)$ preserves the transitions functions. As the domain of the Hamiltonian is determined precisely by these transition functions, we cannot say that $\rho(g)$ preserves the domain. If it does not, we say that G is anomalous [3,4].

More generally, there can be a classical symmetry like parity P which is not part of $\rho(\mathbb{C}G)$. If it does not preserve the domain, that is, the transition functions, then this symmetry is anomalous.

If G is non-abelian, only the elements of G commuting with all $U_{\alpha\beta}$ preserve the domain. The rest are anomalous.

In QCD, the global symmetry group $SU(3)$ can be regarded as the group of constant maps from $\mathbb{R}^3$ to $SU(3)$. Since $SU(3) \cap \mathcal{G}^\infty = \{e\}$, they are not "gauge transformations" as per the considerations hitherto. We should really enlarge $\mathcal{G}^\infty$ to $\mathcal{G}$, which are smooth maps from $\mathbb{R}^3$ to $SU(3)$ which approach a constant value in $SU(3)$ at infinity (that is, when $|\vec{x}| \to \infty$). In that case $SU(3)$ is part of the gauge group. What we have proved in [12–14] is that its action changes the transition functions and hence the domain of the Hamiltonian in the presence of non-abelian monopoles. Hence $SU(3)$ of color is anomalous in the presence of these monopoles.

We conclude this section by listing examples where twisted bundles with non-abelian gauge groups occur. A proper investigation of the physics and mathematics of these bundles from a physical perspective does not exist.

[3]The e_α's after a normalization become orthogonal projectors.
[4]The co-unit for its Hopf algebra [27].

A. Examples

1. From molecular physics

As mentioned above, the rotational degrees of freedom of a molecule are described by the configuration space $Q = SU(2)/G$, where G is a subgroup of $SU(2)$ [20,23]. Since $SU(2) \neq Q \times G$, the principle bundles $G \to SU(2) \to SU(2)/G$ are *all* twisted when $G \neq \{e\}$. There are plenty of molecules with $\rho(G)$ non-abelian.

We will illustrate our general considerations from such Q in the next section.

2. Parastatistics, braid group

The configuration space Q of N identical particles on $\mathbb{R}^d$ is

$$Q = \{[q_1, \ldots, q_N]: q_i \in \mathbb{R}^d, q_i \neq q_j, \quad \text{if } i \neq j\}, \quad (87)$$

where $[q_1, \ldots, q_N]$ is an *unordered* set [20,30,31]:

$$[q_1, q_2, \ldots, q_N] = [q_{s(1)}, q_{s(2)}, \ldots, q_{s(N)}] \quad s \in S_N, \quad (88)$$

S_N being the permutation group of N particles. It is (88) which enforces the particle identity. Thus Q consists of N points of $\mathbb{R}^d$ of cardinality N.

In quantum theory, for $d \geq 3$, the group S_N arises as the "gauge" group commuting with all observables. If $\rho(S_N)$ is abelian, which is the case *only* for bosons and fermions, there is no problem in implementing it on vector states. But if $\rho(S_N)$ is non-abelian, gauge fixing in order to eliminate the redundant vectors in the representation space leads to anomalies.

For $d = 2$, S_N is replaced by the braid group B_N [20,31], allowing the possibility of fractional statistics. Its non-abelian representations have recently occurred in discussions of quantum Hall effect at the filling fraction $\nu = 5/2$ [32], topological quantum computing [33] and the Kitaev model [34]. If $\rho(B_N)$ is non-abelian, it cannot act on properly gauge fixed quantum states.

3. Non-abelian monopoles break color

We have already discussed this issue in Sec. 3 above.

4. Mapping class groups of geons

The mapping class groups here are the groups D^∞/D_0^∞ already defined above for the Friedmann-Sorkin spatial slices supporting topological geons. They are discrete, but are non-abelian for appropriate slices [15–17]. In these cases, if $\rho(D^\infty/D_0^\infty)$ is non-abelian, there might appear quantum diffeo anomalies. We discuss this issue elsewhere [24].

V. ON MOLECULAR CONFIGURATION SPACES

We will adapt the discussion of [23] regarding quantum theories on $Q = SU(2)/G$, with G a subgroup of $SU(2)$ for illustrating our preceding remarks.

Quantization on Q can conveniently start from its universal cover $SU(2)$ and functions on $SU(2)$. The latter are spanned by the components of rotation matrices $D^j_{\lambda\mu}$, with $j \in \mathbb{Z}^+/2$, $\lambda, \mu \in [-j, -j+1, \ldots, j]$, where the scalar product is

$$\langle D^{j'}_{\lambda'\mu'}, D^j_{\lambda\mu}\rangle = \int_{s\in SU(2)} d\mu(s)\bar{D}^{j'}_{\lambda'\mu'}(s)D^j_{\lambda\mu}(s), \quad (89)$$

where $d\mu(s)$ is the invariant $SU(2)$ measure (with volume of $SU(2)$ equal to $16\pi^2$, say). With this scalar product, this space of functions on $SU(2)$ generates a Hilbert space.

On functions f on $SU(2)$, there is a left- and a right-action $U_{L,R}$ of $SU(2)$ defined by

$$(U_L(t)f)(s) = f(t^{-1}s), \quad (90)$$

$$(U_R(t)f)(s) = f(st), \qquad s, t \in SU(2). \quad (91)$$

These actions commute:

$$U_L(s)U_R(t) = U_R(t)U_L(s). \quad (92)$$

The gauge group G and its group algebra $\mathbb{C}G$ act on the *right*, that is, by the representation U_R. The observables lie in $\mathbb{C}U_L(G)$, so that they commute with the gauge transformations $U_R(G)$ and its group algebra $\mathbb{C}U_R(G)$.

We take U_R to be a UIRR. Now,

$$D^j_{\lambda\mu}(st) = D^j_{\lambda\mu'}(s)D^j_{\mu'\mu}(t), \quad (93)$$

so that to obtain an irreducible action of G, we must restrict the second index to a suitable subset.

For example, if $G = \mathbb{Z}_N = \{e^{i(2\pi/N)m\sigma_3}: m = 0, 1, \ldots, N-1\}$, then

$$D^j_{\lambda\mu}(se^{i(2\pi/N)m\sigma_3}) = D^j_{\lambda\mu}(s)e^{i(4\pi/N)m\mu} \quad (94)$$

remembering that μ is associated with eigenvalues for $\sigma_3/2$. So for $\mu \pm 1/2$,

$$e^{i(2\pi/N)\sigma_3} \to e^{\pm i(2\pi/N)}. \quad (95)$$

These two representations may or may not be equivalent depending on N.

For general μ the representations are

$$e^{i(2\pi/N)\sigma_3} \to e^{i(4\pi/N)\mu}. \quad (96)$$

So

$$\mu = \frac{1}{2} + \frac{N}{2}k, \qquad k \in \mathbb{Z} \quad (97)$$

also give the representation

$$e^{i(2\pi/N)\sigma_3} \to e^{+i(2\pi/N)}. \quad (98)$$

For this UIRR, then, the wave functions are spanned by

$$\{D^j_{\lambda,(1/2)+(N/2)k}: k \in \mathbb{Z}\}. \quad (99)$$

For specificity, we focus on the UIRR $e^{i2\pi/N\sigma_3} \to e^{i2\pi/N}$. Using (94), we see that a subset of μ's, call it $\{\nu\}$, carry this UIRR. Then the space spanned by $\{D^j_{\lambda\rho}:\rho \in \{\nu\}\}$ is invariant under observables. We can reduce this further and fix ρ to a particular value $\rho_0 \in \{\nu\}$ or if one prefers, consider the span of $\sum c_\rho D^j_{\lambda\rho}$ for fixed $c_\rho \in \mathbb{C}$.

To present this basis in terms of transition functions, we must cover $SU(2)/G$ by contractible open sets Q_α. Then on Q_α, there is a global section. That is, for $q \in Q_\alpha$, we can pick an element $s_\alpha(q) \in SU(2)$ "in the fiber over" q smoothly. More generally, we can choose a section $s_\alpha(q)g_\alpha(q) \in SU(2)$, with $g_\alpha(q) \in G$.

Now suppose that we choose to work with the span of $D^j_{\lambda\rho_0}(s_\alpha(q)g_\alpha(q))$ over Q_α. Then the sections over Q_α are

$$D^j_{\lambda\rho_0}(s_\alpha(q))U_R(g_\alpha(q)), \tag{100}$$

where $U_R(g_\alpha(q))$ is a phase.

The first factor here corresponds to $|\psi\rangle$ in (78), the second to the factor with σ.

Now consider $U_{\alpha\beta}$. In $U_{\alpha\beta}$, $s_\alpha(q)$ and $s_\beta(q)$ can differ only by the action of the group, so that

$$s_\alpha(q) = s_\beta(q)g_{\beta\alpha}(q), \tag{101}$$

with $q \in Q_\alpha$ and $g_{\beta\alpha}(q) \in G$. Hence

$$D^j_{\lambda\rho_0}(s_\alpha(q))U_R(g_\alpha(q)) = D^j_{\lambda\rho_0}(s_\beta(q))U_R(g_\beta(q)) \times U_R(g_{\beta\alpha}(q)). \tag{102}$$

The last factor $U_R(g_{\beta\alpha}(q))$ regarded as the evaluation at q of a function with values in $U_R(G)$ gives the $U_{\alpha\beta}$ of (84).

In the abelian example, there is no problem of implementing $U_R(g)$ for any $g \in G$, as they preserve the transition functions. Indeed as G is abelian, $G \in \mathcal{C}(\mathbb{C}G)$.

But there can still be classical symmetries which can change $U_{\alpha\beta}$. In particular, parity P and time-reversal T can do so. In [23], it was shown that P and T are *not* violated if and only if

$$U_R(e^{i(4\pi/N)\sigma_3}) = \pm 1. \tag{103}$$

Otherwise they are violated.

The group $\mathbb{Z}_N$ occurs as G (called H^* in [23]) for pyramidal molecules. There are pyramidal molecules where (103) is not fulfilled. Their quantum theories violate P and T. But just like QCD, PT is not anomalous in quantum theories.

The groups D^*_{4N}, with $N \in \mathbb{Z}$, is the gauge group G for "staggered" and "eclipsed" configurations such as those of ethane [23].

The group D^*_8 has the following elements:

$$D^*_8 = \{\pm 1, \pm i\tau_i\} \subset SU(2). \tag{104}$$

It is the "symmetry group" or the gauge group leaving the shape of the biaxial nematic invariant.

Reference [23] shows that molecules with N even do not violate P or T.

But D^*_{4N} are all non-abelian for $N \geq 2$. If D^*_{4N} has K UIRR's, then the center $\mathcal{C}(\mathbb{C}D^*_{4N})$ is of dimension K. For a generic UIRR U_R, only $U_R(e_\alpha)$, $e_\alpha \in \mathcal{C}(\mathbb{C}D^*_{4N})$ and their linear combinations are well-defined in a quantum theory, and we cannot implement the UIRR's U_R of D^*_{4N}.

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