





THE WAVE FUNCTIONAL  
FOR THE GAUGE FIELD  
& CP VIOLATION/CONSERVATION

BJÖRN GARBRECHT

Technische Universität München

Bethe Forum "Axions"

UNI BONN, OCTOBER 11TH, 2022



Collaborators  
WEN-YUAN AI  
JUAN CRUZ  
CARLOS TAMARIT

## Two problems for strong $CP$ : Topological quantization and the first postulate of QM

- Fermion correlations  
(from the path integral, this time using instantons)  
As for topological quantization
- Theta vacua and wave functionals (in canonical quantization)  
As for the first postulate of QM (normalizable states)

# Two problems for strong $CP$ : Topological quantization and the first postulate of QM

- **Fermion correlations**

(from the path integral, this time using instantons)

As for topological quantization

- Theta vacua and wave functionals (in canonical quantization)

As for the first postulate of QM (normalizable states)

## Fermion correlations: Setup

$CP$ -odd Lagrangian terms in the strong interactions:

$$\mathcal{L} \supset - \sum_{j=1}^{N_f} \bar{\psi}_j m_j e^{i\alpha_j \gamma^5} \psi_j + \frac{1}{16\pi^2} \theta \operatorname{tr} F_{\mu\nu} \tilde{F}^{\mu\nu}$$

Chiral symmetry of the fermions is anomalous  $\longrightarrow$

Rephasing invariant:  $\bar{\theta} = \theta + \bar{\alpha}$ , where  $\bar{\alpha} = \sum_{j=1}^{N_f} \alpha_j$ ,  $\longrightarrow \theta$  is an angle  
[Fujikawa (1979,80)]

Theta-term/topological term is a total divergence

$$\frac{1}{4} \operatorname{tr} F_{\mu\nu} \tilde{F}^{\mu\nu} = \partial_\mu K_\mu \quad K_\mu = \epsilon_{\mu\nu\alpha\beta} \operatorname{tr} \left[ \frac{1}{2} A_\nu \partial_\alpha A_\beta + \frac{1}{3} A_\nu A_\alpha A_\beta \right]$$

Instantons: Surface term does not vanish at infinity

Winding number/topological charge:

$$\Delta n = \frac{1}{16\pi^2} \int d^4x F_{\mu\nu} \tilde{F}^{\mu\nu} = \frac{1}{4\pi^2} \oint_{S^3} d^3\sigma K_\perp$$

## Boundary configurations for the path integral

The parameter  $\theta$  can be viewed as an angular variable (forced by the anomalous chiral current).  $\longrightarrow$

Requires  $\Delta n \in \mathbb{Z}$  (“topological quantization”)  $\rightarrow \exp(iS)|_{\theta} = \exp(iS)|_{\theta+2\pi}$

**Readily built into the path integral without constraining boundary conditions by hand:**

(Relatively) nonvanishing contributions in *infinite* spacetime only from classical saddle points and fluctuations about these

Vanishing physical fields on the boundary of the infinite spacetime volume ( $VT \rightarrow \infty$ ) are the only boundary configurations leading to **saddle points with finite Euclidean action in  $\mathbb{R}^4$**

( $\equiv$  multi-instanton solutions to the EOMs). [*cf.* Coleman (1985)]

*There is no such restriction/principle to fixed physical bcs. for finite  $VT$ .*

Indeed, for pure gauge configurations  $\rightarrow \Delta n \in \mathbb{Z}$

**Consequence:** In the path integral, sum over all topological sectors  $\Delta n$ , weigh these by  $\exp(i\Delta n\theta)$

## Effective 't Hooft vertex

Instanton effects described by effective 't Hooft vertex: [t Hooft (1976,86)]

$$\mathcal{L} + \frac{1}{16\pi^2} \theta \operatorname{tr} F_{\mu\nu} \tilde{F}^{\mu\nu} \rightarrow \mathcal{L} - \Gamma_{N_f} e^{i\xi} \prod_{j=1}^{N_f} (\bar{\psi}_j P_L \psi_j) - \Gamma_{N_f} e^{-i\xi} \prod_{j=1}^{N_f} (\bar{\psi}_j P_R \psi_j)$$

( $\Gamma_{N_f}$  some coefficient)

$\xi$  should be expressed in terms of parameters of the fundamental theory

Two options:

$$\begin{aligned} \xi = \theta \quad (\text{in general misaligned with masses}) &\quad \rightarrow CP \text{ violation} \\ \xi = -\bar{\alpha} \quad (\text{present claim, aligned with mass terms}) &\quad \rightarrow \text{no } CP \text{ violation} \end{aligned}$$

Note: For both  $\bar{\theta}$  remains the only rephasing invariant  $CP$  phase

Both comply with  $\chi$ ral anomaly

$$\left. \begin{aligned} \prod_{j=1}^{N_f} \psi_j &\rightarrow \prod_{j=1}^{N_f} e^{i\beta\gamma_5} \psi_j, & \prod_{j=1}^{N_f} \bar{\psi}_j &\rightarrow \prod_{j=1}^{N_f} \bar{\psi}_j e^{i\beta\gamma_5} \\ \bar{\alpha} &\rightarrow \bar{\alpha} - 2N_f\beta, & \theta &\rightarrow \theta + 2N_f\beta, & \bar{\theta} &\rightarrow \bar{\theta} \end{aligned} \right\} \text{For invariant } \mathcal{L}$$

In principle, we could have  $\xi = c_\alpha \bar{\alpha} + c_\theta \theta$  for integer  $c_{\alpha, \theta}$  ( $\alpha, \theta$  are angular variables) with  $c_\alpha + c_\theta = 1$ . We shall see that this general case is not realized in the explicit calculation.

The effective vertex is chosen so that it generates the following **correlation functions** at tree level:

$$\langle \prod_{j=1}^{N_f} \psi_j(x_j) \bar{\psi}_j(x'_j) \rangle_{\text{inst}} = \left( e^{-i\xi} \prod_{j=1}^{N_f} P_{Lj} + e^{i\xi} \prod_{j=1}^{N_f} P_{Rj} \right) \bar{H}(x_1, \dots, x'_1, \dots)$$

Cf. leading contribution to two-point function

$$\langle \psi_i(x) \psi_j(x') \rangle = i S_{0\text{inst } ij}(x, x')$$
$$i S_{0\text{inst } ij}(x, x') = (-\gamma^\mu \partial_\mu + i m_i e^{-i\alpha_i \gamma^5}) \int \frac{d^4 p}{(2\pi)^4} e^{-ip(x-x')} \frac{\delta_{ij}}{p^2 - m_i^2 + i\epsilon}$$

So  $\xi = \theta/\xi = -\bar{\alpha}$  implies *CP*-violation/no *CP*-violation

Take  $N_f = 1$  from here onwards

Calculations e.g. of neutron EDM implicitly *assume*  $\xi = \theta$

[e.g. Baluni (1979); Crewther, Di Vecchia, Veneziano, Witten (1979)]

## Fermion correlations in DIG approximation

### Before coming with instantons

Generally know (chiral anomaly):  $\theta$  should be angular

If the partition function  $Z$  is analytic in  $\theta$ , then the minimum of the potential  $V(\theta)$  is parity even. [Vafa, Witten (1986)]

Relating  $\chi$  to  $V(\theta)$  relies on analyticity of  $Z$  in  $\theta \longrightarrow$  Analyticity valid?

Explicit derivations of  $V(\theta) \sim \cos \theta$

[Callan, Dashen, Gross (1976)]

Thus far only calculation of strong  $CP$  violation in quarks by [t Hooft (1986)]

} These rely on dilute instanton gas (DIG) approximation

While semiclassical methods do not apply to strongly coupled models, it is reasonable to believe that the outcome of strong  $CP$  and  $U(1)_A$  is determined by topological/instanton effects.

In turn: If the strong  $CP$  problem does not show up in the DIG, then there is a problem for the strong  $CP$  problem.

DIG  $\longrightarrow$  intuitive insight into quark  $CP$  (non)conservation

## Plan of the calculation

To obtain fermion correlation functions:

- Green's functions in instanton backgrounds
- Interferences within topological sectors
- Interference between the sectors  
(where the order of  $\sum_{-\infty}^{\infty} \Delta n$  and  $VT \rightarrow \infty$  matters)

## Green's functions for fermions

Euclidean Green's function  $S^E(x^E, x^{E'})$  satisfies

$$(\not{D}^E + m_R + i\gamma^5 m_I)S^E(x^E, x^{E'}) = \delta^4(x^E - x^{E'})$$

Spectral sum (first massless case):

$$\begin{aligned} \not{D}^E \hat{\psi}_\lambda^E &= \left( \not{\partial}^E + \gamma_m^E A_m^E \right) \hat{\psi}_\lambda^E = \lambda^E \hat{\psi}_\lambda^E \\ \longrightarrow S^E(x^E, x^{E'}) &= \sum_{\lambda^E} \frac{\hat{\psi}_\lambda^E(x^E) \hat{\psi}_\lambda^{E\dagger}(x^{E'})}{\lambda^E} \end{aligned}$$

Spectral sum for  $m = 0$  is ill-defined because of the fermionic zero mode  $\lambda^E = 0$  in the instanton background

**Euclidean index theorem:**  $\Delta n$  equals difference between number of right-handed and left-handed zero modes

→ One left (right)-handed zero-mode for  $\Delta n = -1$  ( $\Delta n = 1$ )

Left-handed zero mode [t Hooft (1976)]

$$\hat{\psi}_{0L}^E(x^E) = \begin{pmatrix} \chi_0^E(x^E) \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix}, \quad \text{where } \chi_0^E(x^E) = \frac{\varrho u}{\pi [\varrho^2 + (x^E)^2]^{\frac{3}{2}}}, \quad u^{\alpha b} = \varepsilon^{\alpha b}$$

Include mass @ first order in perturbation theory ( $\Delta n = -1$  background) [Shifman, Vainshtein, Zakharov (1979)]

$$S^E(x^E, x^{E'}) = \frac{\hat{\psi}_0^E(x^E)\hat{\psi}_0^{E\dagger}(x^{E'})}{me^{-i\alpha}} + \sum_{\lambda^E \neq 0} \frac{\hat{\psi}_\lambda^E(x^E)\hat{\psi}_\lambda^{E\dagger}(x^{E'})}{\lambda^E}$$

## Green's function in $n$ -instanton, $\bar{n}$ -anti-instanton background

$$iS_{n,\bar{n}}(x, x') \approx iS_{0\text{inst}}(x, x') + \sum_{\bar{\nu}=1}^{\bar{n}} \frac{\varphi_{0L}(x - x_{0,\bar{\nu}})\varphi_{0L}^\dagger(x' - x_{0,\bar{\nu}})}{m e^{-i\alpha}} + \sum_{\nu=1}^n \frac{\varphi_{0R}(x - x_{0,\nu})\varphi_{0R}^\dagger(x' - x_{0,\nu})}{m e^{i\alpha}}$$

Comments:

- For small masses, zero-modes dominate close to the cores of the instantons, far away from the instantons the solution goes to the zero-instanton configuration [Diakonov, Petrov (1986)]
- **Alignment** of phase  $\alpha$  between Lagrangian mass and instanton-induced  $\chi\text{SB}$   $\rightarrow$  No indication of  $CP$  violation here
- Should be expected— $\theta$ -phase has not entered calculation thus far

## Green's function in $n$ -instanton, $\bar{n}$ -anti-instanton background

$$iS_{n,\bar{n}}(x, x') \approx iS_{0\text{inst}}(x, x') + \sum_{\bar{\nu}=1}^{\bar{n}} \frac{\varphi_{0L}(x - x_{0,\bar{\nu}})\varphi_{0L}^\dagger(x' - x_{0,\bar{\nu}})}{me^{-i\alpha}} + \sum_{\nu=1}^n \frac{\varphi_{0R}(x - x_{0,\nu})\varphi_{0R}^\dagger(x' - x_{0,\nu})}{me^{i\alpha}}$$

cf.

$$iS_{0\text{inst}}(x, x') = (-\gamma^\mu \partial_\mu + ime^{-i\alpha} \gamma^5) \int \frac{d^4 p}{(2\pi)^4} e^{-ip(x-x')} \frac{1}{p^2 - m^2 + i\epsilon}$$

instantons, far away from the instantons the solution goes to the zero-instanton configuration [Diakonov, Petrov (1986)]

- **Alignment** of phase  $\alpha$  between Lagrangian mass and instanton-induced  $\chi$ SB  $\rightarrow$  No indication of  $CP$  violation here
- Should be expected— $\theta$ -phase has not entered calculation thus far

## Green's function in $n$ -instanton, $\bar{n}$ -anti-instanton background

$$iS_{n,\bar{n}}(x, x') \approx iS_{0\text{inst}}(x, x') + \sum_{\bar{\nu}=1}^{\bar{n}} \frac{\varphi_{0L}(x - x_{0,\bar{\nu}})\varphi_{0L}^\dagger(x' - x_{0,\bar{\nu}})}{m e^{-i\alpha}} + \sum_{\nu=1}^n \frac{\varphi_{0R}(x - x_{0,\nu})\varphi_{0R}^\dagger(x' - x_{0,\nu})}{m e^{i\alpha}}$$

Comments:

- For small masses, zero-modes dominate close to the cores of the instantons, far away from the instantons the solution goes to the zero-instanton configuration [Diakonov, Petrov (1986)]
- **Alignment** of phase  $\alpha$  between Lagrangian mass and instanton-induced  $\chi\text{SB}$   $\rightarrow$  No indication of  $CP$  violation here
- Should be expected— $\theta$ -phase has not entered calculation thus far

## Interferences within the topological sectors

Within a topological sector, interfere/sum/integrate over

- all instanton/anti-instanton numbers  $n + \bar{n}$  with  $\Delta n = n - \bar{n}$  fixed
- locations of all instantons/anti-instantons
- remaining collective coordinates

Evaluate correlation and partition function first for **fixed**  $\Delta n$

$$\begin{aligned}
 & \langle \psi(x) \bar{\psi}(x') \rangle_{\Delta n} \\
 &= \sum_{\substack{\bar{n}, n \geq 0 \\ n - \bar{n} = \Delta n}} \int \mathcal{D}A_{\bar{n}, n} \mathcal{D}\bar{\psi} \mathcal{D}\psi \psi(x) \bar{\psi}(x') e^{-S_E[A, \bar{\psi}, \psi]} \\
 &= \sum_{\substack{\bar{n}, n \geq 0 \\ n - \bar{n} = \Delta n}} \frac{1}{\bar{n}! n!} \left( \prod_{\bar{\nu}=1}^{\bar{n}} \int_{V_T} d^4 x_{0, \bar{\nu}} d\Omega_{\bar{\nu}} J_{\bar{\nu}} \right) \left( \prod_{\nu=1}^n \int_{V_T} d^4 x_{0, \nu} d\Omega_{\nu} J_{\nu} \right) iS_{\bar{n}, n}(x, x') \\
 & \quad \times e^{-S_E(\bar{n}+n)} e^{-i(\bar{n}-n)(\alpha+\theta)} (-\Theta \varpi)^{(\bar{n}+n)}
 \end{aligned}$$

$\mathcal{D}A_{\bar{n}, n}$ : Gauge field fluctuations about saddle with  $n$  instantons,  $\bar{n}$  anti-instantons

$d\Omega_{\nu} J_{\nu}$ : Non-translational zero modes & Jacobians for all zero modes

$\Theta, \varpi$ : Reduced fermion & gauge/ghost determinants in instanton background

$iS_{\bar{n}, n}(x, x')$ : Fermion propagator in  $n$  instantons,  $\bar{n}$  anti-instanton background

$S_E[A, \bar{\psi}, \psi]$ : Full action functional

$S_E$ : Euclidean action for one (anti-)instanton

Likewise, partition function:

$$\begin{aligned}
 Z_{\Delta n} &= \sum_{\substack{\bar{n}, n \geq 0 \\ n - \bar{n} = \Delta n}} \int \mathcal{D}A_{\bar{n}, n} \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S_E[A, \bar{\psi}, \psi]} \\
 &= \sum_{\substack{\bar{n}, n \geq 0 \\ n - \bar{n} = \Delta n}} \frac{1}{\bar{n}! n!} \left( -\int d\Omega J V T \Theta \varpi e^{-S_E} \right)^{(\bar{n}+n)} e^{-i(\bar{n}-n)(\alpha+\theta)}
 \end{aligned}$$

## Integrate out locations of the instanton

$$\begin{aligned} & \int_{VT} d^4x_{0,\bar{\nu}} iS(x, x') \\ & \approx \int_{VT} d^4x_{0,\bar{\nu}} \left[ iS_{0\text{inst}}(x, x') + \frac{\varphi_{0\text{L}}(x - x_{0,\bar{\nu}})\varphi_{0\text{L}}^\dagger(x' - x_{0,\bar{\nu}})}{me^{-i\alpha}} + \dots \right] \\ & = VT (iS_{0\text{inst}}(x, x') + \dots) + m^{-1}e^{i\alpha}h(x, x')P_{\text{L}} \end{aligned}$$

Dots represent contributions from the zero modes of the (anti)-instantons whose centres were not integrated over

$h(x, x')$  is defined as a block-diagonal matrix (with two identical blocks):

$$\begin{aligned} h(x, x')P_{\text{L}} &= \int_{VT} d^4x_{0,\bar{\nu}} \varphi_{0\text{L}}(x - x_{0,\bar{\nu}})\varphi_{0\text{L}}^\dagger(x' - x_{0,\bar{\nu}}) \\ h(x, x')P_{\text{R}} &= \int_{VT} d^4x_{0,\bar{\nu}} \varphi_{0\text{R}}(x - x_{0,\bar{\nu}})\varphi_{0\text{R}}^\dagger(x' - x_{0,\bar{\nu}}) \\ \bar{h}(x, x') &\equiv \frac{\int d\Omega h(x, x')}{\int d\Omega} \end{aligned}$$

Integrating over all locations  $\longrightarrow$  Correlation function for fixed  $\Delta n$ :

$$\begin{aligned} & \langle \psi(x) \bar{\psi}(x') \rangle_{\Delta n} \\ &= \sum_{\substack{\bar{n}, n \geq 0 \\ n - \bar{n} = \Delta n}} \frac{1}{\bar{n}! n!} \left[ \bar{h}(x, x') \left( \frac{\bar{n}}{m e^{-i\alpha}} P_L + \frac{n}{m e^{i\alpha}} P_R \right) (VT)^{\bar{n}+n-1} + i S_{0\text{inst}}(x, x') (VT)^{\bar{n}+n} \right] \\ & \qquad \qquad \qquad \times (i\kappa)^{\bar{n}+n} (-1)^{n+\bar{n}} e^{i\Delta n(\alpha+\theta)} \\ &= \left[ \left( e^{i\alpha} I_{\Delta n+1}(2i\kappa VT) P_L + e^{-i\alpha} I_{\Delta n-1}(2i\kappa VT) P_R \right) \frac{i\kappa}{m} \bar{h}(x, x') + I_{\Delta n}(2i\kappa VT) i S_{0\text{inst}}(x, x') \right] \\ & \qquad \qquad \qquad \times (-1)^{\Delta n} e^{i\Delta n(\alpha+\theta)} \end{aligned}$$

where  $i\kappa = \int d\Omega J \Theta \varpi e^{-S_E}$  and  $I_\nu(x)$  is the modified Bessel function

Sum is dominated by particular value of  $n \approx \bar{n}$ : [Diakonov, Petrov (1986)]

$$\langle n \rangle = \frac{\sum_{n=0}^{\infty} n \frac{(\kappa VT)^n}{n!}}{\sum_{n=0}^{\infty} \frac{(\kappa VT)^n}{n!}} = \kappa VT, \quad \frac{\sqrt{\langle (n - \langle n \rangle)^2 \rangle}}{\langle n \rangle} = \frac{1}{\sqrt{\kappa VT}}$$

Cf.  $\lim_{x \rightarrow \infty} I_{\Delta n}(ix e^{-i0^+}) / I_{\Delta n'}(ix e^{-i0^+}) = 1$

$\longrightarrow$  No relative  $CP$  phase between mass and instanton induced breaking of  $\chi$ ral symmetry—**alignment** in infinite-volume limit

Correspondingly, partition function for fixed  $\Delta n$ : [cf. Leutwyler, Smilga (1992)]

$$Z_{\Delta n} = I_{\Delta n}(2i\kappa VT) (-1)^{\Delta n} e^{i\Delta n(\alpha+\theta)}$$

**Note:** The topological phase  $e^{i\Delta n(\alpha+\theta)}$  multiplies  $\langle \psi(x)\bar{\psi}(x') \rangle_{\Delta n}$  and  $Z_{\Delta n}$  entirely—not just the contributions induced by instantons.

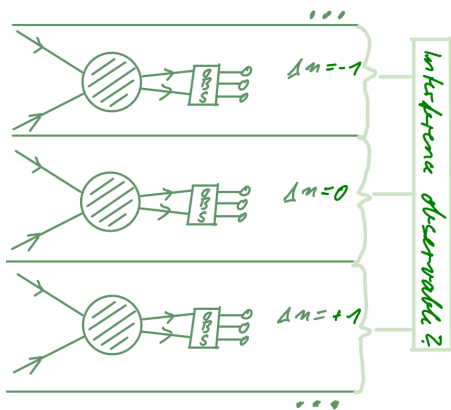
Other correlation functions ( $n$  point, stress-energy, for some observer,...) are calculated from the Feynman diagram with the Green's function in the  $n$  instanton,  $\bar{n}$  anti-instanton background.

Then it remains to average over  $n$ ,  $\bar{n}$ , locations and remaining collective coordinates.

There is no  $CP$  violation/misalignment of phases to this end. It remains to consider the interference between the topological sectors.

## Can interference between topological sectors be observed?

- Effective action well-defined for each sector separately—barriers of infinite action separate sectors of different  $\Delta n$
- Possible to observe the interference between the topological sectors of different  $\Delta n$ ? **Superobserver?**



Topological phases  $e^{i\Delta n(\alpha+\theta)}$  appear globally for each topological sector. An observer made up of local quantum fields cannot access separate sectors.

Anyway: Turns out interferences are immaterial in the limit  $VT \rightarrow \infty$

# Interferences among topological sectors (are immaterial)

Topological quantization  $\leftrightarrow$  Interference between sectors for  $VT \rightarrow \infty$

## Fermion correlator

$$\begin{aligned}\langle \psi(x) \bar{\psi}(x') \rangle &= \lim_{\substack{N \rightarrow \infty \\ N \in \mathbb{N}}} \lim_{VT \rightarrow \infty} \frac{\sum_{\Delta n = -N}^N \langle \psi(x) \bar{\psi}(x') \rangle_{\Delta n}}{\sum_{\Delta n = -N}^N Z_{\Delta n}} \\ &= iS_{0\text{inst}}(x, x') + i\kappa \bar{h}(x, x') m^{-1} e^{-i\alpha\gamma^5} \quad (\text{same as for fixed } \Delta n)\end{aligned}$$

$$\text{Recall: } iS_{0\text{inst}}(x, x') = (-\gamma^\mu \partial_\mu + ime^{-i\alpha\gamma^5}) \int \frac{d^4 p}{(2\pi)^4} e^{-ip(x-x')} \frac{1}{p^2 - m^2 + i\epsilon}$$

$\longrightarrow$  No relative  $CP$ -phase between mass and instanton term

## Limits ordered the other way around

First sum over all  $\Delta n$  as well:

$$\begin{aligned} & \sum_{\bar{n}, n \geq 0} \frac{1}{\bar{n}! n!} \left[ \bar{h}(x, x') (\bar{n} m^{-1} e^{i\alpha} P_L + n m^{-1} e^{-i\alpha} P_R) (VT)^{\bar{n}+n-1} + iS_{0\text{inst}}(x, x') (VT)^{\bar{n}+n} \right] \\ & \qquad \qquad \qquad \times (-mi\kappa)^{\bar{n}+n} e^{i\Delta n(\alpha+\theta)} \\ & = \left[ - \left( e^{-i\theta} P_L + e^{i\theta} P_R \right) \frac{i\kappa}{m} \bar{h}(x, x') + iS_{0\text{inst}}(x, x') \right] e^{-2i\kappa VT \cos(\alpha+\theta)} \end{aligned}$$

$$Z \rightarrow \sum_{n, \bar{n}} \frac{1}{n! \bar{n}!} (-i\kappa VT)^{\bar{n}+n} e^{-i(\bar{n}-n)(\alpha+\theta)} = e^{-2i\kappa VT \cos(\alpha+\theta)}$$

Then,  $VT \rightarrow \infty$  trivial as  $VT$ -dependence cancels

→ Relative  $CP$  phase leading to  $CP$ -violating observables

However: The order of limits is not a choice but dictated by the fact that boundary conditions for the topological sectors are imposed at infinity.

Quantum mechanical systems: For a finite number of degenerate minima, there is only a finite number of classes of tunneling transitions.

→ Order of limits not an issue

Two problems for strong  $CP$ :

Topological quantization and the first postulate of QM

- Fermion correlations

(from the path integral, this time using instantons)

As for topological quantization

- **Theta vacua and wave functionals** (in canonical quantization)

As for the first postulate of QM (normalizable states)

## Theta vacuum, standard story

The action & path integral are a first-principle definition of the theory. However, vacuum states (i.e. field functionals) are sometimes used.

Consider initial and final states, taking  $x_4 \rightarrow \pm\infty$

→ Construct from pure gauge configurations on these surfaces, with

$$\Delta n = \frac{1}{16\pi^2} \int d^4x F_{\mu\nu} \tilde{F}_{\mu\nu} = n_\infty - n_{-\infty} \quad \text{gauge invariant}$$

$$n_{\pm\infty} = \frac{1}{4\pi^2} \int_{x^4=\pm\infty} d^3\sigma K_\perp \quad \text{Chern-Simons number, **not** gauge invariant}$$

Gauge transformations  $\Omega$  change  $n_{\pm\infty}$  by same number of integer units

Construct ground states from prevacua:  $n_{-\infty} \rightarrow |n\rangle$   
 $n_\infty \rightarrow \langle n|$  (field eigenstates)

Gauge invariant (up to phase) state  $|\theta\rangle = \sum_n e^{-in\theta} |n\rangle$

[Callan, Dashen, Gross (1976); Jackiw, Rebbi (1976); Jackiw (1980)]

## Two shortcomings

The prevacua  $|n\rangle$  are field eigenstates, very different from the ground state

Resolutions:

- Take  $T \rightarrow \infty$  in the path integral to project on the ground state:  
 $|\text{vac}\rangle = e^{-HT} \sum_n e^{-in\theta} |n\rangle$ ,  $T \rightarrow \infty$  (cf.  $VT \rightarrow \infty$  in previous part)
- Or construct a wave functional [Jackiw, Rebbi (1976); Jackiw (1980)]

States are not normalizable in the proper sense because  
 $\langle \theta | \theta' \rangle = \delta(\theta - \theta')$  [cf. e.g. Callan, Dashen, Gross (1970); issue taken by Okubo, Marshak (1992)]

Without ado, this contradicts 1st postulate of quantum mechanics.

Possible resolutions:

- Construct wave packets—not acceptable however because gauge invariance should be exact
- Use gauge fixing in order to normalize states—to be discussed in this talk

## Two shortcomings

The prevacua  $|n\rangle$   
ground state

Resolutions:

- Take  $T \rightarrow \infty$   
 $|\text{vac}\rangle = e^{-HT}$
- Or construct a

States are not normalized  
 $\langle \theta | \theta' \rangle = \delta(\theta - \theta')$

Without ado, this contradicts 1st postulate of quantum mechanics.

Possible resolutions:

- Construct wave packets—not acceptable however because gauge invariance should be exact
- Use gauge fixing in order to normalize states—to be discussed in this talk

### B. STATEMENT OF THE POSTULATES

#### 1. Description of the state of a system

In chapter I, we introduced the concept of the quantum state of a particle. We first characterized this state at a given time by a square-integrable wave function. Then, in chapter II, we associated a ket of the state space  $\mathcal{E}_r$  with each wave function: choosing  $|\psi\rangle$  belonging to  $\mathcal{E}_r$  is equivalent to choosing the corresponding function  $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$ . Therefore, the quantum state of a particle at a fixed time is characterized by a ket of the space  $\mathcal{E}_r$ . In this form, the concept of a state can be generalized to any physical system.

*First Postulate:* At a fixed time  $t_0$ , the state of a physical system is defined by specifying a ket  $|\psi(t_0)\rangle$  belonging to the state space  $\mathcal{E}$ .

[Cohen-Tanoudji, Diu, Laloë]

## Two shortcomings

The prevacua  $|n\rangle$  are field eigenstates, very different from the ground state

Resolutions:

- Take  $T \rightarrow \infty$  in the path integral to project on the ground state:  
 $|\text{vac}\rangle = e^{-HT} \sum_n e^{-in\theta} |n\rangle$ ,  $T \rightarrow \infty$  (cf.  $VT \rightarrow \infty$  in previous part)
- Or construct a wave functional [Jackiw, Rebbi (1976); Jackiw (1980)]

States are not normalizable in the proper sense because  
 $\langle \theta | \theta' \rangle = \delta(\theta - \theta')$  [cf. e.g. Callan, Dashen, Gross (1970); issue taken by Okubo, Marshak (1992)]

Without ado, this contradicts 1st postulate of quantum mechanics.

Possible resolutions:

- Construct wave packets—not acceptable however because gauge invariance should be exact
- Use gauge fixing in order to normalize states—to be discussed in this talk

## Canonical quantization of the gauge field

Minkowski spacetime, no sources  $\longrightarrow$

$$g\vec{E}^a = -\partial/\partial t \vec{A}^a$$

$$g\vec{B}^a = \nabla \times \vec{A}^a - 1/2 f^{abc} \vec{A}^a \times \vec{A}^b$$

Canonical momentum conjugate to  $\vec{A}^a$ :

$$g\vec{\Pi}^a = -\vec{E}^a + \frac{g^2}{8\pi^2} \theta \vec{B}^a$$

The corresponding operator must observe the commutation relations:

$$[A^{a,i}(\vec{x}), \Pi^{b,j}(\vec{x}')] = i\delta^{ij} \delta^{ab} \delta^3(\vec{x} - \vec{x}'), \quad [\Pi^{a,i}(\vec{x}), \Pi^{b,j}(\vec{x}')] = 0$$

These commutators hold for ( $\theta_\Pi$  arbitrary)  $\vec{\Pi}^a = \frac{\delta}{i\delta\vec{A}^a} + \theta_\Pi \frac{g}{8\pi^2} \vec{B}^a$ .

Hamiltonian density:

$$\mathcal{H} = \frac{1}{2} \left( (\vec{E}^a)^2 + (\vec{B}^a)^2 \right) = \frac{1}{2} \left( \left( g \frac{\delta}{i\delta\vec{A}^a} - \frac{g^2}{8\pi^2} (\theta - \theta_\Pi) \vec{B}^a \right)^2 + (\vec{B}^a)^2 \right)$$

## Wave functional in gauge theory

$\mathcal{G}_n$ : “large” gauge transformation that changes the Chern–Simons number by  $n$  units

Since  $[\mathcal{G}_n, \mathcal{H}] = 0$ , it is possible to find states/wave functionals that simultaneously satisfy

$$\begin{aligned}\mathcal{H}\Psi &= E\Psi \\ \mathcal{G}_n\Psi(\vec{A}^a) &= e^{in\theta'}\Psi(\vec{A}^a)\end{aligned}$$

States with this property constitute subspaces invariant under the action of the Hamiltonian, i.e.  $\theta'$  is protected by a superselection rule.

(NB:  $\theta'$  is independent of  $\theta$  in the Lagrangian and  $\theta_\Pi$  in the canonical momentum)

## Abstract formulation

Wave function(al):  $\Psi(\vec{V})$

Let  $T$  be a translation of  $\vec{V}$  that corresponds to a unitary operator  $G(T)$  acting on  $\Psi$ :

$$\Psi(T\vec{V}) = G(T)\Psi(\vec{V})$$

Eigensystem of  $G(T)$ :

$$\begin{aligned}\Psi_\theta(T\vec{V}) &= e^{i\theta}\Psi_\theta(\vec{V}) \Rightarrow \\ \Psi_\theta(T^n\vec{V}) &= G^n(T)\Psi_\theta(\vec{V}) = e^{in\theta}\Psi_\theta(\vec{V}) \quad \text{for integer } n\end{aligned}$$

(The correspondence is:  $\vec{V} \leftrightarrow \vec{A}^a$ ,  $G^n(T) \leftrightarrow \mathcal{G}_n$ )

Define a function  $N(\vec{V})$  with the property  $N(T\vec{V}) = N(\vec{V}) + 1$

$$\begin{aligned}\longrightarrow \Psi_\theta(\vec{V}) &= \psi_\theta(\vec{V})e^{iN(\vec{V})\theta} \\ \longrightarrow \Psi_\theta(T\vec{V}) &= \psi_\theta(\vec{V})e^{i(N(\vec{V})+1)\theta}\end{aligned}$$

where  $\psi_\theta$  is periodic in  $T$ :

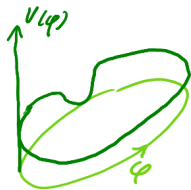
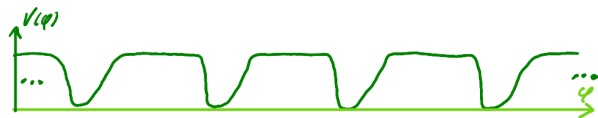
$$\psi_\theta(T\vec{V}) = e^{-iN(T\vec{V})\theta}\Psi_\theta(T\vec{V}) = e^{-i(N(\vec{V})+1)\theta}e^{i\theta}\Psi_\theta(\vec{V}) = e^{-iN(\vec{V})\theta}\Psi_\theta(\vec{V}) = \psi_\theta(\vec{V})$$

## Crystal or circle?

Let  $H(T\vec{V}) = H(\vec{V})$ . The functionals  $\Psi_\theta(\vec{V})$  with above periodicity properties can be viewed as Bloch states.

Bloch states live on a crystal:

$T\vec{V}$  is a *different* site than  $\vec{V}$



In contrast: In gauge theory  $T\vec{V}$  is a *redundant* description of the configuration  $\vec{V}$ —corresponding to  $\varphi \rightarrow \varphi + 2\pi n$  on a circle

[see e.g. Shifman, *Advanced QFT* (2012)]

On a crystal: Bloch states do not correspond to normalized wave functions, these are rather wave packets made up of Bloch states.

On a circle: Truncation of the inner product according to a single period leads to properly normalizable states, corresponding to *gauge fixing*:

$$\int_{0 \leq N(\vec{V}) < 1} d\vec{V} \Psi^*(\vec{V}) \Psi(\vec{V}) = 1, \quad \langle \mathcal{O} \rangle = \int_{0 \leq N(\vec{V}) < 1} d\vec{V} \Psi^*(\vec{V}) \mathcal{O} \Psi(\vec{V})$$

## Quantum states on a circle

Quantization on a single period appears to resolve the issue of improperly normalizable states and also seems to be appropriate in view of the physical redundancy of gauge field configurations.

Surely, the spectrum on a circle should differ from one in a crystal. But how and why exactly?

Essence of the problem is captured by particle on a circle, angular coordinate  $\varphi$ , gauge transformation  $T^n \varphi = \varphi + 2\pi n$

Lagrangian:

$$L = \frac{1}{2} m R^2 (\dot{\varphi} + \omega)^2 + \mathcal{V}(\varphi)$$

$2\omega\dot{\varphi}$  is a total derivative corresponding to a  $\theta$ -term

Canonical momentum:  $\pi_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = m R^2 (\dot{\varphi} + \omega)$

Hamiltonian:  $H = \pi_\varphi \dot{\varphi} - L = \frac{1}{2} \frac{1}{m R^2} (\pi_\varphi - m R^2 \omega)^2 - \frac{1}{2} m R^2 \omega^2 + \mathcal{V}(\varphi)$

Momentum operator:  $[\varphi, \pi_\varphi] = i \Rightarrow \pi_\varphi = -i \partial_\varphi - m R^2 \omega_B$

# Galilei transformation on a circle

## Unitary operator for boosts

Now take  $\pi = -i\partial_\varphi$  for definiteness

$$U(\omega_b) = e^{i\omega_b M} \text{ where } M = \pi t - mR^2\varphi$$

$$\pi \mapsto \pi' = \pi + mR^2\omega_b \qquad U(\omega_b)\varphi U^\dagger(\omega_b) = \varphi + \omega_b t$$

$$\varphi \mapsto \varphi' + \omega_b t \qquad U(\omega_b)\pi U^\dagger(\omega_b) = \pi + mR^2\omega_b$$

$$U(\omega_b)\psi(\varphi) = e^{-imR^2\omega_b\varphi} e^{-i\frac{mR^2\omega_b^2 t}{2}} \psi(\varphi + \omega_b t)$$

## Periodicity condition

Hamiltonian

$$H = \frac{1}{2} \frac{1}{mR^2} \left( \frac{1}{i} \partial_\varphi - mR^2 \omega \right)^2 + \mathcal{V}(\varphi)$$

For  $\omega = 0$ ,  $\psi(\varphi) = \psi(\varphi + 2\pi n)$  appears to be the correct periodicity condition (cf. embedding of the circle in two dimensions)

However:

- Galilei-boosts lead more generally to  $\psi(\varphi) = e^{-2\pi i n m R^2 \omega \theta} \psi(\varphi + 2\pi n)$
- Invariance of QM expectation values under  $\varphi \rightarrow \varphi + 2\pi n$  likewise only requires periodicity up to a phase
- Space is not necessarily simply connected

What is the physical/mathematical interpretation of the less general periodicity and how to generalize it to  $\omega \neq 0$ ?

## Consistent time evolution

Heisenberg equation for operator  $\mathcal{O}(\exp(i\varphi))$ :

$$\begin{aligned} [H, \mathcal{O}(e^{i\varphi})] &= \frac{d}{dt} \mathcal{O}(e^{i\varphi}) = \frac{1}{2mR^2} \left[ \left( \frac{1}{i} \frac{\partial}{\partial \varphi} - mR^2 \omega \right)^2, \mathcal{O}(e^{i\varphi}) \right] \\ &= -\frac{1}{2mR^2} \left( \frac{\partial^2}{\partial \varphi^2} \mathcal{O}(e^{i\varphi}) \right) - \frac{1}{mR^2} \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \frac{\partial}{\partial \varphi} - i\omega \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \end{aligned}$$

→

$$\Phi(\varphi) e^{i\varphi m R^2 \omega} [H, \mathcal{O}(e^{i\varphi})] e^{-i\varphi m R^2 \omega} \Phi(\varphi) = -\frac{1}{2} \frac{\partial}{\partial \varphi} \Phi(\varphi) \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \Phi(\varphi)$$

For energy-eigenstate wave-functions that work for the truncated inner product:

$$0 = \langle d/dt \mathcal{O}(e^{i\varphi}) \rangle = \int_{0 \leq \varphi < 2\pi} d\varphi \psi^*(\varphi) (d/dt \mathcal{O}(e^{i\varphi})) \psi(\varphi)$$

→

$$\psi(\varphi) = e^{-imR^2\omega\varphi} \Phi(\varphi) \quad \text{where} \quad \Phi(\varphi) \in \mathbb{R} \quad \text{and} \quad \Phi(\varphi) = \Phi(\varphi + 2\pi)$$

Then, the integrand is a total derivative, and boundary terms vanish by the periodicity of  $\Phi(\varphi)$ .

## Consistent time evolution

Heisenberg equation for operator  $\mathcal{O}(e^{i\varphi})$ :

Eigensystem of Hamiltonian:

$$\left[ \begin{array}{l} H \\ \text{For } \omega = 0 \text{ in } H \Rightarrow \psi(\varphi) = \psi(\varphi + 2\pi n) \\ \text{For } \omega \neq 0 \text{ in } H \Rightarrow \psi(\varphi) = e^{2\pi i n m R^2 \omega} \psi(\varphi + 2\pi n) \\ \text{so that the } \omega\text{-phases compensate, i.e. they can} \\ \text{be simultaneously removed from } H \text{ and } \psi \text{ by a} \\ \text{Galilean transformation} \end{array} \right] \begin{array}{l} e^{i\varphi} \\ \\ \\ \\ \\ (e^{i\varphi}) \end{array}$$

$$\rightarrow \Phi(\varphi) e^{i\varphi m R^2 \omega} [H, \mathcal{O}(e^{i\varphi})] e^{-i\varphi m R^2 \omega} \Phi(\varphi) = -\frac{1}{2} \frac{\partial}{\partial \varphi} \Phi(\varphi) \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \Phi(\varphi)$$

For energy-eigenstate wave-functions that work for the truncated inner product:

$$0 = \langle d/dt \mathcal{O}(e^{i\varphi}) \rangle = \int_{0 \leq \varphi < 2\pi} d\varphi \psi^*(\varphi) (d/dt \mathcal{O}(e^{i\varphi})) \psi(\varphi)$$

$$\rightarrow \psi(\varphi) = e^{-imR^2\omega\varphi} \Phi(\varphi) \quad \text{where} \quad \Phi(\varphi) \in \mathbb{R} \quad \text{and} \quad \Phi(\varphi) = \Phi(\varphi + 2\pi)$$

Then, the integrand is a total derivative, and boundary terms vanish by the periodicity of  $\Phi(\varphi)$ .

## Consistent time evolution

Heisenberg equation for operator  $\mathcal{O}(\exp(i\varphi))$ :

$$\begin{aligned} [H, \mathcal{O}(e^{i\varphi})] &= \frac{d}{dt} \mathcal{O}(e^{i\varphi}) = \frac{1}{2mR^2} \left[ \left( \frac{1}{i} \frac{\partial}{\partial \varphi} - mR^2 \omega \right)^2, \mathcal{O}(e^{i\varphi}) \right] \\ &= -\frac{1}{2mR^2} \left( \frac{\partial^2}{\partial \varphi^2} \mathcal{O}(e^{i\varphi}) \right) - \frac{1}{mR^2} \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \frac{\partial}{\partial \varphi} - i\omega \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \end{aligned}$$

→

$$\Phi(\varphi) e^{i\varphi m R^2 \omega} [H, \mathcal{O}(e^{i\varphi})] e^{-i\varphi m R^2 \omega} \Phi(\varphi) = -\frac{1}{2} \frac{\partial}{\partial \varphi} \Phi(\varphi) \left( \frac{\partial}{\partial \varphi} \mathcal{O}(e^{i\varphi}) \right) \Phi(\varphi)$$

For energy-eigenstate wave-functions that work for the truncated inner product:

$$0 = \langle d/dt \mathcal{O}(e^{i\varphi}) \rangle = \int_{0 \leq \varphi < 2\pi} d\varphi \psi^*(\varphi) (d/dt \mathcal{O}(e^{i\varphi})) \psi(\varphi)$$

→

$$\psi(\varphi) = e^{-imR^2\omega\varphi} \Phi(\varphi) \quad \text{where} \quad \Phi(\varphi) \in \mathbb{R} \quad \text{and} \quad \Phi(\varphi) = \Phi(\varphi + 2\pi)$$

Then, the integrand is a total derivative, and boundary terms vanish by the periodicity of  $\Phi(\varphi)$ .

## Physics picture

Take  $H = -\frac{1}{2} \frac{1}{mR^2} \partial_\varphi^2 + \mathcal{V}(\varphi)$  ( $\omega = 0$  can always be achieved by boosts)

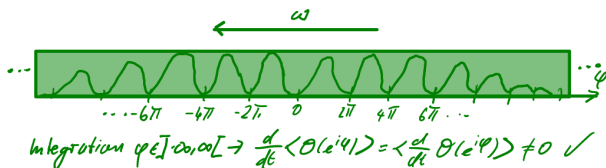
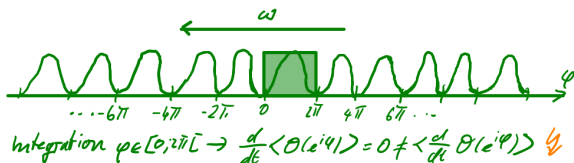
$\psi(\varphi) = e^{2\pi i n m R^2 \omega} \psi(\varphi + 2\pi n) \rightarrow$  wave with crystal momentum  $\propto \omega$

Schrödinger equation is to be solved on the full range  $\varphi \in \mathbb{R}$

Truncation of the inner product is only consistent with operator equations of motion for wave functions with  $\omega = 0$

For  $\omega \neq 0$  consistent time evolution follows for *normalizable wave packets*—these are not fully invariant under discrete translations

(large gauge transformations), and their overall hull moves in time



## Back to gauge theory

For the Hamiltonian

$$\mathcal{H} = \frac{1}{2} \left( (\vec{E}^a)^2 + (\vec{B}^a)^2 \right) = \frac{1}{2} \left( \left( g \frac{\delta}{i\delta\vec{A}^a} - \frac{g^2}{8\pi^2} \theta \vec{B}^a \right)^2 + (\vec{B}^a)^2 \right)$$

The wave functionals with the property  $\mathcal{G}_n \Psi(\vec{A}^a) = e^{-in\theta} \Psi(\vec{A}^a)$  are the only ones that are consistent with time evolution, gauge invariance and that are properly normalizable.

These exhibit no  $CP$  violation ( $\theta$  can be *simultaneously* boosted away from Hamiltonian and wave functional):

$$K(\vec{A}^a) = \frac{1}{8\pi^2} \epsilon^{ijk} \int d^3x \left( \frac{1}{2} A^{a,i} \partial_j A^{a,k} - \frac{1}{6} f^{abc} A^{a,i} A^{b,j} A^{c,k} \right)$$

$$\Psi'(\vec{A}^a) = e^{i\theta K(\vec{A}^a)} \Psi(\vec{A}^a) \Rightarrow \mathcal{G}_n \Psi' = \Psi'$$

$$\mathcal{H}' = e^{i\theta K(\vec{A}^a)} \mathcal{H} e^{-i\theta K(\vec{A}^a)} = \frac{1}{2} \left( -g^2 \frac{\delta^2}{\delta\vec{A}^a{}^2} + (\vec{B}^a)^2 \right)$$

## Conclusion

There is no  $CP$ -violation in QCD with massive quarks.

Based on challenges to standard calculations:

- **Path integral**

What would be the reason to impose topological quantization on a *finite* surface? Integer topological sectors only follow in *infinite spacetime* (save periodic boundary conditions), the latter can be viewed as a tool to project on the ground state.

- **Theta vacua:**

The description of the vacuum by states that are not properly normalizable is in contradiction with the postulates of QM. Gauge fixing leads to normalizable states, and consistent QM time evolution in the canonical formalism requires the restriction to  $CP$ -conserving theories.

The background of the image consists of a pair of red curtains with vertical folds, creating a textured, draped appearance. The lighting is slightly brighter in the center, highlighting the texture of the fabric.

**THANK YOU!**

## Topological term

Theta-term/topological term is a total divergence

$$\frac{1}{4} \text{tr} F_{\mu\nu} \tilde{F}_{\mu\nu} = \partial_\mu K_\mu \quad K_\mu = \epsilon_{\mu\nu\alpha\beta} \text{tr} \left[ \frac{1}{2} A_\nu \partial_\alpha A_\beta + \frac{1}{3} A_\nu A_\alpha A_\beta \right]$$

→ Equivalent to a surface term, i.e. the flux of the current through the boundary of the integration volume

So does it vanish?

Cf. anti-instanton:  $A_\mu^u{}_v = -\frac{\sigma_{\mu\nu}^u x_\nu}{x^2 + \rho^2}$  (extended solution to Euclidean EOMs) [Belavin, Polyakov, Schwarz, Tyupkin (1975)]

Surface term decays as  $1/|x|^3 \rightarrow$  surface integral does not need to vanish

For  $x^2 \rightarrow \infty$ , the instanton field becomes a pure gauge:

$$A_\mu \rightarrow -\frac{i}{g}(\partial_\mu \Omega)\Omega^{-1} \quad \text{where } \Omega \in \text{SU}(2)$$

$$K_\mu \rightarrow \frac{1}{6}\varepsilon_{\mu\nu\lambda\rho}\text{tr}[(\Omega^{-1}\partial_\nu\Omega)(\Omega^{-1}\partial_\lambda\Omega)(\Omega^{-1}\partial_\rho\Omega)]$$

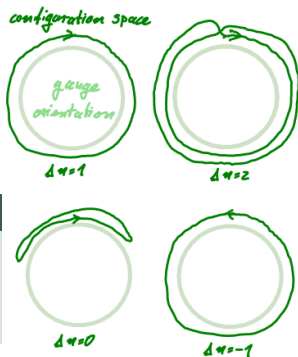
Winding number—topological quantization

$$\Delta n = \frac{1}{16\pi^2} \int d^4x F_{\mu\nu} \tilde{F}_{\mu\nu} = \frac{1}{4\pi^2} \oint_{S^3} d^3\sigma K_\perp$$

Integrand is a Haar measure and maps  $S^3 \rightarrow S^3$

(Anti-)instanton is a configuration with winding number  $\Delta n = (-)1$

Theta term contributes to the action though being a total derivative



## Effective operators

Effective interactions in the theory with fermions (present analysis)

→ Effective operators in  $\chi$ ral perturbation theory

→ Observables such as neutron EDM,  $\eta' \rightarrow \pi\pi$

$VT \rightarrow \infty$  before  $\sum_{\Delta n}$

$$\mathcal{L} \rightarrow \mathcal{L} - \bar{\psi}(x)\Gamma e^{i\alpha\gamma^5}\psi(x)$$

Alignment with  $\bar{\psi}m \exp(i\alpha\gamma^5)\psi$

No  $CP$ -violating observables

$\sum_{\Delta n}$  before  $VT \rightarrow \infty$

$$\mathcal{L} \rightarrow \mathcal{L} + \bar{\psi}(x)\Gamma e^{-i\theta\gamma^5}\psi(x)$$

Misaligned with  $\bar{\psi}m \exp(i\alpha\gamma^5)\psi$

$CP$ -violating observables

$$N_f \text{ flavours: } \mathcal{L} \rightarrow \mathcal{L} - \Gamma_{N_f} e^{-i\bar{\alpha}} \prod_{j=1}^{N_f} (\bar{\psi}_j P_L \psi_j) - \Gamma_{N_f} e^{i\bar{\alpha}} \prod_{j=1}^{N_f} (\bar{\psi}_j P_R \psi_j)$$

## Effective chiral Lagrangian

$$U = U_0 e^{\frac{i}{f_\pi} \Phi} \quad \text{chiral condensate}$$

$$\Phi = \begin{bmatrix} \pi^0 + \frac{1}{\sqrt{3}}\eta + \sqrt{\frac{2}{3}}\eta' & \sqrt{2}\pi^+ & \sqrt{2}K^+ \\ \sqrt{2}\pi^- & -\pi^0 + \frac{1}{\sqrt{3}}\eta + \sqrt{\frac{2}{3}}\eta' & \sqrt{2}K^0 \\ \sqrt{2}K^- & \sqrt{2}\bar{K}^0 & -\frac{2}{\sqrt{3}}\eta + \sqrt{\frac{2}{3}}\eta' \end{bmatrix}$$

Chiral Lagrangian (lowest order terms):

$$\mathcal{L} = \frac{f_\pi^2}{4} \text{Tr} \partial_\mu U \partial^\mu U^\dagger + \frac{f_\pi^2 B_0}{2} \text{Tr}(MU + U^\dagger M^\dagger) \\ + |\lambda| e^{-i\xi} f_\pi^4 \det U + |\lambda| e^{i\xi} f_\pi^4 \det U^\dagger$$

Consider  $M$ ,  $|\lambda|e^{i\xi}$  as symmetry breaking *sources*. There are

- $U(3)_A$  invariant terms
- $U(3)_A$  breaking terms depending on the same parameter  $M = \text{diag}\{m_u e^{i\alpha_u}, m_d e^{i\alpha_d}, m_s e^{i\alpha_s}\}$  as the quark masses in the fundamental theory (systematic construction by promotion of  $M$  to a spurion)
- $U(1)_A$  breaking terms depending on the parameter  $|\lambda|e^{i\xi}$

## Now which is $\xi$ in the effective chiral Lagrangian?

Transformation of  $U$  under chiral field redefinitions:

$$\arg U = \arg \langle \bar{\psi}(x) P_R \psi(x) \rangle \Rightarrow U \rightarrow e^{2i\beta} U \Rightarrow \det U \rightarrow e^{2iN_f\beta} \det U$$

Further the Lagrangian then remains invariant with

$$\theta \rightarrow \theta + 2N_f\beta \quad \text{so that} \quad \bar{\alpha} \rightarrow \bar{\alpha} - 2N_f\beta$$

→

Both,  $\xi = -\bar{\alpha}$  or  $\xi = \theta$  once more comply with the chiral anomaly and leave  $\bar{\theta} = \theta + \bar{\alpha}$  rephasing invariant. The high energy theory must tell us which is  $\xi$ .

The 't Hooft operator—which transforms under chiral rotations in the same way as  $\det U$ —comes with  $e^{i\xi} = e^{-i\bar{\alpha}}$  (given the correct order of limits).

So we have to set  $\xi = -\bar{\alpha}$ , by the same logic that leads to the identification of  $M$  with the quark masses.

## VI. Finite sub(volumes)

Boundary conditions at infinity crucial for alignment of the  $CP$  phases

Calculations in finite spacetime volumes should also be possible

- for subvolumes of spacetime ( $\rightarrow$  open boundary conditions),
- for periodic boundary conditions, e.g. on a torus as in lattice field simulations.

Note: On a torus,  $\Delta n$  is topologically conserved.

Lattice simulations sample over  $\Delta n$  because of finite lattice spacing.

Topology “freezes” in the continuum limit.

## Finite vs infinite spacetime volume—cluster decomposition

Consider expectation value of an operator  $\mathcal{O}$  in spacetime volume  $\Omega$ , interfere different topological sectors  $\Delta n$ : [Weinberg QFT]

$$\langle \mathcal{O} \rangle_{\Omega} = \lim_{\substack{N \rightarrow \infty \\ N \in \mathbb{N}}} \frac{\sum_{\Delta n = -N}^N f(\Delta n) \int_{\Delta n} \mathcal{D}\phi \mathcal{O} e^{-S_{\Omega}[\phi]}}{\sum_{\Delta n = -N}^N f(\Delta n) \int_{\Delta n} \mathcal{D}\phi e^{-S_{\Omega}[\phi]}}$$

Factorize path integral into volume contributions,  $\Omega = \Omega_1 \cup \Omega_2$ :

$$\begin{aligned} \langle \mathcal{O}_1 \rangle_{\Omega} &= \lim_{\substack{N_2 \rightarrow \infty \\ N_2 \in \mathbb{N}}} \lim_{\substack{N_1 \rightarrow \infty \\ N_1 \in \mathbb{N}}} \quad (\text{Assume } \Delta n(\Omega) = \Delta n_1(\Omega_1) + \Delta n_2(\Omega_2)) \\ &= \frac{\sum_{\Delta n_1 = -N_1}^{N_1} \sum_{\Delta n_2 = -N_2}^{N_2} f(\Delta n_1 + \Delta n_2) \int_{\Delta n_1} \mathcal{D}\phi \mathcal{O}_1 e^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2} \mathcal{D}\phi e^{-S_{\Omega_2}[\phi]}}{\sum_{\Delta n_1 = -N_1}^{N_1} \sum_{\Delta n_2 = -N_2}^{N_2} f(\Delta n_1 + \Delta n_2) \int_{\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2} \mathcal{D}\phi e^{-S_{\Omega_2}[\phi]}} \end{aligned}$$

Independence of  $\langle \mathcal{O}_1 \rangle_{\Omega}$  from the fluctuations in  $\Omega_2$  is achieved if the contributions from  $\Omega_2$  cancel (absorb determinant phases in  $f$ ):

$$f(\Delta n_1 + \Delta n_2) = f(\Delta n_1) f(\Delta n_2) \Rightarrow f(\Delta n) = e^{i\Delta n(\alpha + \theta)}$$

Now keep  $\Delta n$  fixed,  $\Omega_2$  either finite or infinite:

$$\begin{aligned}
 \langle \mathcal{O}_1 \rangle_\Omega &= \frac{\sum_{\Delta n_1=-\infty}^{\infty} f(\Delta n) \int_{\Delta n_1} \mathcal{D}\phi \mathcal{O}_1 e^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2=\Delta n-\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_2}[\phi]}}{\sum_{\Delta n_1=-\infty}^{\infty} f(\Delta n) \int_{\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2=\Delta n-\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_2}[\phi]}} \\
 &= \frac{\sum_{\Delta n_1=-\infty}^{\infty} f(\Delta n) I_{\Delta n-\Delta n_1}(2i\kappa\Omega_2) \int_{\Delta n_1} \mathcal{D}\phi \mathcal{O}_1 e^{-S_{\Omega_1}[\phi]}}{\sum_{\Delta n_1=-\infty}^{\infty} f(\Delta n) I_{\Delta n-\Delta n_1}(2i\kappa\Omega_2) \int_{\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_1}[\phi]}} \\
 &\underset{\Omega_2 \gg \Omega_1}{\approx} \frac{\sum_{\Delta n_1=-\infty}^{\infty} \int_{\Delta n_1} \mathcal{D}\phi \mathcal{O}_1 e^{-S_{\Omega_1}[\phi]}}{\sum_{\Delta n_1=-\infty}^{\infty} \int_{\Delta n_1} \mathcal{D}\phi e^{-S_{\Omega_1}[\phi]}}
 \end{aligned}$$

Corresponds to  
finite  $VT$ ,  $\theta = 0$

Result also holds for  
 $\Omega_2 \rightarrow \infty$ ,  $\Delta n$  free



Path integral makes sense for finite subvolumes with open boundary conditions  
 $\hat{=}$  lattice simulations sampling over topological sectors  $\Delta n$  *without* phases

The theory with fixed  $\Delta n$  (gauge invariant) in large but finite volumes **complies with cluster decomposition** [cf. Leutwyler, Smilga (1992)]. Lattice results with frozen topology are therefore okay up to finite volume effects.

For  $\Omega_2 \rightarrow \infty$ , the result does not depend on whether  $\Delta n$  is fixed or free.

Title image: <https://web.archive.org/web/20161023012858/http://www.panoramio.com/photo/60013307>

License: <https://creativecommons.org/licenses/by-sa/3.0/deed.en>