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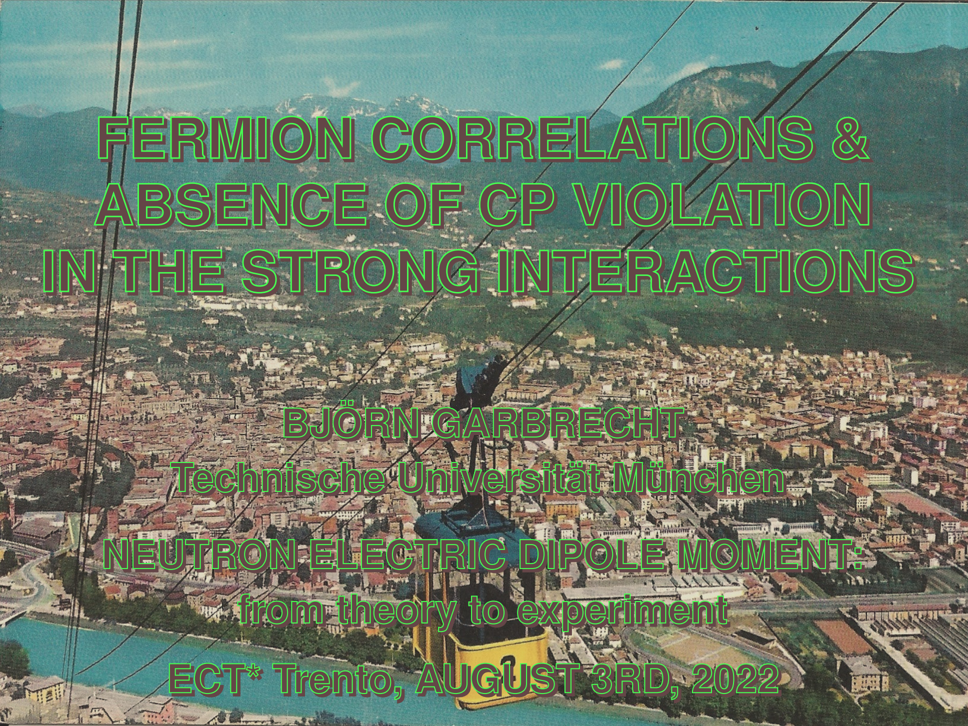

FERMION CORRELATIONS & ABSENCE OF CP VIOLATION IN THE STRONG INTERACTIONS

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NEUTRON ELECTRIC DIPOLE MOMENT:
from theory to experiment

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Two parts

- Fermion correlations (from the path integral)
- Theta vacua and wave functionals (in canonical quantization)

Outline: Fermion correlations

I. CP-odd Lagrangians, correlations & effective operators
CP-odd invariants in QCD and potentially related observables
$\rightarrow$ *Fermion correlations*

II. Topological term
Path integral, boundary configurations, integer topological charges

III. Green's functions for fermions
Euclidean Green's function in fixed instanton background

IV. Interferences within the topological sectors
Integration over collective coordinates, e.g. instanton locations, leads to correlation functions in a fixed topological sector

V. Interferences among different topological sectors (are immaterial)
Taking the infinite-volume limit before summing over the topological sectors, there is alignment of the chiral CP phases in the fermion sector

I. CP-odd Lagrangians, correlations & effective operators

CP-odd Lagrangian terms in the strong interactions:

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

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

Effective 't Hooft vertex

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

$$\mathcal{L} + \frac{1}{16\pi^2}\theta\,\mathrm{tr}F_{\mu\nu}\tilde{F}^{\mu\nu} \to \mathcal{L} - \Gamma_{N_f}\mathrm{e}^{\mathrm{i}\xi}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{L}}\psi_j) - \Gamma_{N_f}\mathrm{e}^{-\mathrm{i}\xi}\prod_{j=1}^{N_f}(\bar{\psi}_j P_{\mathrm{R}}\psi_j)$$

(Γ_{N_f} some coefficient)

ξ should be expressed in terms of parameters of the fundamental theory

Two options:

$\xi = \theta$ (in general misaligned with masses) $\to$ CP violation

$\xi = -\bar{\alpha}$ (present claim, aligned with mass terms) $\to$ no CP violation

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

Both comply with χral anomaly

$$\prod_{j=1}^{N_f}\psi_j \to \prod_{j=1}^{N_f}\mathrm{e}^{\mathrm{i}\beta\gamma_5}\psi_j, \quad \prod_{j=1}^{N_f}\bar{\psi}_j \to \prod_{j=1}^{N_f}\bar{\psi}_j\,\mathrm{e}^{\mathrm{i}\beta\gamma_5}$$

$$\bar{\alpha} \to \bar{\alpha} - 2N_f\beta, \quad \theta \to \theta + 2N_f\beta, \quad \bar{\theta} \to \bar{\theta}$$

In principle, we could have $\xi = c_\alpha\bar{\alpha} + c_\theta\theta$ for integer $c_{\alpha,\theta}$ (α, θ 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:

$$\langle\prod_{j=1}^{N_f}\psi_j(x_j)\bar{\psi}_j(x_j')\rangle_{\rm inst} = \left(\mathrm{e}^{-\mathrm{i}\xi}\prod_{j=1}^{N_f}P_{\mathrm{L}j} + \mathrm{e}^{\mathrm{i}\xi}\prod_{j=1}^{N_f}P_{\mathrm{R}j}\right)\bar{H}(x_1,\ldots,x_1',\ldots)$$

Cf. leading contribution to two-point function

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

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)]

Only one explicit calculation based on dilute instanton gas finding $\xi = \theta$
['t Hooft (1986)]

II. Topological term

Theta-term/topological term is a total divergence

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

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

So does it vanish?

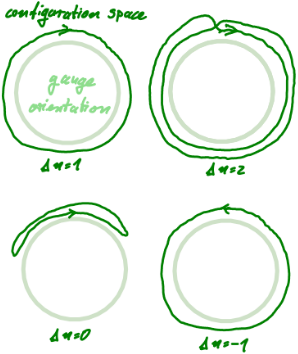
Cf. anti-instanton: $A_\mu{}^u{}_v = -\frac{\sigma_{\mu\nu}{}^u{}_v x_\nu}{x^2+\rho^2}$ (extended solution to Euclidean EOMs) [Belavin, Polyakov, Schwarz, Tyupkin (1975)]

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

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

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

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



Winding number—topological quantization

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

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

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

Theta term contributes to the action though being a total derivative

Boundary configurations for the path integral

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

Requires $\Delta n \in \mathbb{Z}$ ("topological quantization") $\rightarrow \exp(\mathrm{i}S)|_\theta = \exp(\mathrm{i}S)|_{\theta+2\pi}$

This is readily built into the path integral:
(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 for finite VT.

Indeed, for pure gauge configurations $\rightarrow \Delta n \in \mathbb{Z}$ (as discussed above)

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

III. Green's functions for fermions

Goal: Fermion correlations

Plan of calculation

- Obtain correlation functions from Green's functions in fixed background of instantons and anti-instantons
- Interfere all instanton configurations
  - First, within one topological sector
  - Then over the different sectors

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

$$(\not{D}^{\mathrm{E}} + m_{\mathrm{R}} + \mathrm{i}\gamma^5 m_{\mathrm{I}}) S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime}) = \delta^4(x^{\mathrm{E}} - x^{\mathrm{E}\prime})$$

Spectral sum (first massless case):

$$\not{D}^{\mathrm{E}} \hat{\psi}^{\mathrm{E}}_{\lambda} = \left(\not{\partial}^{\mathrm{E}} + \gamma^{\mathrm{E}}_{m} A^{\mathrm{E}}_{m}\right) \hat{\psi}^{\mathrm{E}}_{\lambda} = \lambda^{\mathrm{E}} \hat{\psi}^{\mathrm{E}}_{\lambda}$$

$$\longrightarrow \quad S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime}) = \sum\!\!\!\!\!\!\!\int_{\lambda^{\mathrm{E}}} \frac{\hat{\psi}^{\mathrm{E}}_{\lambda}(x^{\mathrm{E}}) \hat{\psi}^{\mathrm{E}\dagger}_{\lambda}(x^{\mathrm{E}\prime})}{\lambda^{\mathrm{E}}}$$

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

Euclidean index theorem: Δn equals difference between number of right-handed and left-handed zero modes

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

Left-handed zero mode ['t Hooft (1976)]

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

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

$$S^{\mathrm{E}}(x^{\mathrm{E}}, x^{\mathrm{E}\prime}) = \frac{\hat{\psi}^{\mathrm{E}}_0(x^{\mathrm{E}})\hat{\psi}^{\mathrm{E}\dagger}_0(x^{\mathrm{E}\prime})}{m e^{-\mathrm{i}\alpha}} + \sum\!\!\!\!\!\!\!\int_{\lambda^{\mathrm{E}}\neq 0} \frac{\hat{\psi}^{\mathrm{E}}_\lambda(x^{\mathrm{E}})\hat{\psi}^{\mathrm{E}\dagger}_\lambda(x^{\mathrm{E}\prime})}{\lambda^{\mathrm{E}}}$$

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

$$
\begin{aligned}
\mathrm{i}S_{n,\bar{n}}(x,x') \approx \mathrm{i}S_{0\mathrm{inst}}(x,x') &+ \sum_{\bar{\nu}=1}^{\bar{n}} \frac{\varphi_{0\mathrm{L}}(x-x_{0,\bar{\nu}})\varphi^{\dagger}_{0\mathrm{L}}(x'-x_{0,\bar{\nu}})}{m\mathrm{e}^{-\mathrm{i}\alpha}} \\
&+ \sum_{\nu=1}^{n} \frac{\varphi_{0\mathrm{R}}(x-x_{0,\nu})\varphi^{\dagger}_{0\mathrm{R}}(x'-x_{0,\nu})}{m\mathrm{e}^{\mathrm{i}\alpha}}
\end{aligned}
$$

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 α between Lagrangian mass and instanton-induced χSB $\longrightarrow$ No indication of CP violation here
- Should be expected—θ-phase has not entered calculation thus far

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

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

cf.

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

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IV. 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

$\longrightarrow$ Dilute instanton gas approximation

Can also obtain coincident fermion correlations using the index theorem and anomalous current only

Evaluate correlation and partition function first for **fixed** Δn

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

$\mathcal{D}A_{\bar n,n}$:	Gauge field fluctuations about saddle with n instantons, $\bar n$ anti-instantons
$\mathrm{d}\Omega_\nu J_\nu$:	Non-translational zero modes & Jacobians for all zero modes
Θ,ϖ :	Reduced fermion & gauge/ghost determinants in instanton background
$\mathrm{i}S_{\bar n,n}(x,x')$:	Fermion propagator in n instantons, $\bar n$ anti-instanton background
$S_{\mathrm{E}}[A,\bar\psi,\psi]$:	Full action functional
S_{E}:	Euclidean action for one (anti-)instanton

Likewise, partition function:

$$Z_{\Delta n} = \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \int \mathcal{D}A_{\bar{n},n}\mathcal{D}\bar{\psi}\mathcal{D}\psi\, \mathrm{e}^{-S_{\mathrm{E}}[A,\bar{\psi},\psi]}$$

$$= \sum_{\substack{\bar{n},n\geq 0\\ n-\bar{n}=\Delta n}} \frac{1}{\bar{n}!n!} \left(-\textstyle\int \mathrm{d}\Omega\, J\, V T\, \Theta\, \varpi\, \mathrm{e}^{-S_{\mathrm{E}}}\right)^{(\bar{n}+n)} \mathrm{e}^{-\mathrm{i}(\bar{n}-n)(\alpha+\theta)}$$

Integrate out locations of the instanton

$$\begin{aligned}
&\int_{VT} \mathrm{d}^4 x_{0,\bar\nu}\ \mathrm{i}S(x,x') \\
&\approx \int_{VT} \mathrm{d}^4 x_{0,\bar\nu} \left[\mathrm{i}S_{0\mathrm{inst}}(x,x') + \frac{\varphi_{0\mathrm{L}}(x-x_{0,\bar\nu})\varphi^{\dagger}_{0\mathrm{L}}(x'-x_{0,\bar\nu})}{m\mathrm{e}^{-\mathrm{i}\alpha}} + \cdots \right] \\
&= VT\left(\mathrm{i}S_{0\mathrm{inst}}(x,x') + \cdots\right) + m^{-1}\mathrm{e}^{\mathrm{i}\alpha} h(x,x') P_{\mathrm{L}}
\end{aligned}$$

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):

$$h(x,x')P_{\mathrm{L}} = \int_{VT} \mathrm{d}^4 x_{0,\bar\nu}\, \varphi_{0\mathrm{L}}(x-x_{0,\bar\nu})\varphi^{\dagger}_{0\mathrm{L}}(x'-x_{0,\bar\nu})$$

$$h(x,x')P_{\mathrm{R}} = \int_{VT} \mathrm{d}^4 x_{0,\bar\nu}\, \varphi_{0\mathrm{R}}(x-x_{0,\bar\nu})\varphi^{\dagger}_{0\mathrm{R}}(x'-x_{0,\bar\nu})$$

$$\bar{h}(x,x') \equiv \frac{\int d\Omega\, h(x,x')}{\int d\Omega}$$

Integrating over all locations ⟶ Correlation function for fixed Δn:

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

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

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

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

Cf. $\lim_{x\to\infty}I_{\Delta n}(\mathrm{i}x\,\mathrm{e}^{-\mathrm{i}0^+})/I_{\Delta n'}(\mathrm{i}x\,\mathrm{e}^{-\mathrm{i}0^+})=1$

⟶ No relative CP phase between mass and instanton induced breaking of χral symmetry—**alignment** in infinite-volume limit

Correspondingly, partition function for fixed Δn: [cf. Leutwyler, Smilga (1992)]

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

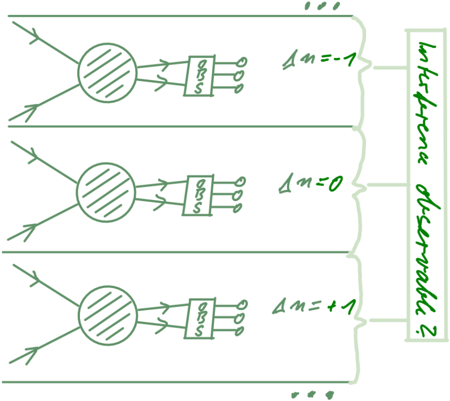
Note: The topological phase $\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}$ multiplies $\langle\psi(x)\bar{\psi}(x')\rangle_{\Delta n}$ and $Z_{\Delta n}$ entirely—not just the contributions induced by instantons.

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 Δn
- Possible to observe the interference between the topological sectors of different Δn? **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 $VT \to \infty$

V. Interferences among topological sectors (are immaterial)

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

Fermion correlator

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

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

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

Limits ordered the other way around

First sum over all Δn as well:

$$\sum_{\bar{n},n\geq 0}\frac{1}{\bar{n}!n!}\Big[\bar{h}(x,x')(\bar{n}\,m^{-1}\mathrm{e}^{\mathrm{i}\alpha}P_{\mathrm{L}}+n\,m^{-1}\mathrm{e}^{-\mathrm{i}\alpha}P_{\mathrm{R}})\,(VT)^{\bar{n}+n-1}+\mathrm{i}S_{0\mathrm{inst}}(x,x')\,(VT)^{\bar{n}+n}\Big] \times(-mi\kappa)^{\bar{n}+n}\mathrm{e}^{\mathrm{i}\Delta n(\alpha+\theta)}$$

$$=\left[-\left(\mathrm{e}^{-\mathrm{i}\theta}P_{\mathrm{L}}+\mathrm{e}^{\mathrm{i}\theta}P_{\mathrm{R}}\right)\frac{\mathrm{i}\kappa}{m}\bar{h}(x,x')+\mathrm{i}S_{0\mathrm{inst}}(x,x')\right]\mathrm{e}^{-2\mathrm{i}\kappa VT\cos(\alpha+\theta)}$$

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

Then, $VT\to\infty$ trivial as VT-dependence cancels
$\longrightarrow$ 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.
$\to$ Order of limits not an issue

Effective operators

Effective interactions in the theory with fermions (present analysis)
$\longrightarrow$ Effective operators in χral perturbation theory
$\longrightarrow$ Observables such as neutron EDM, $\eta' \to \pi\pi$

$VT \to \infty$ **before** $\sum_{\Delta n}$	$\sum_{\Delta n}$ **before** $VT \to \infty$
$\mathcal{L} \to \mathcal{L} - \bar{\psi}(x)\Gamma \mathrm{e}^{\mathrm{i}\alpha\gamma^5}\psi(x)$	$\mathcal{L} \to \mathcal{L} + \bar{\psi}(x)\Gamma \mathrm{e}^{-\mathrm{i}\theta\gamma^5}\psi(x)$
Alignment with $\bar{\psi} m \exp(\mathrm{i}\alpha\gamma^5)\psi$	Misaligned with $\bar{\psi} m \exp(\mathrm{i}\alpha\gamma^5)\psi$
No CP-violating observables	CP-violating observables

N_f flavours: $\mathcal{L} \to \mathcal{L} - \Gamma_{N_f} \mathrm{e}^{-\mathrm{i}\bar{\alpha}} \prod_{j=1}^{N_f} (\bar{\psi}_j P_{\mathrm{L}} \psi_j) - \Gamma_{N_f} \mathrm{e}^{\mathrm{i}\bar{\alpha}} \prod_{j=1}^{N_f} (\bar{\psi}_j P_{\mathrm{R}} \psi_j)$

Effective chiral Lagrangian

$U = U_0 \mathrm{e}^{\frac{\mathrm{i}}{f_\pi}\Phi}$ 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):

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

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

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

Now which is ξ in the effective chiral Lagrangian?

Transformation of U under chiral field redefinitions:

$$\arg U = \arg\langle\bar{\psi}(x)P_{\mathrm{R}}\psi(x)\rangle \;\Rightarrow\; U \to \mathrm{e}^{2\mathrm{i}\beta}U \;\Rightarrow\; \det U \to \mathrm{e}^{2\mathrm{i}N_f\beta}\det U$$

Further the Lagrangian then remains invariant with

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

$\longrightarrow$

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 ξ.

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

Outline: Theta vacua and wave functionals

I. Theta vacuum, standard story
   Superposition of an infinite number of field eigenstates & its open ends

II. Canonical quantization of the gauge field
   Wave functional representation of the state; gauge redundancy

III. Quantum states on a circle
   How the spectrum for a potential on a circle is different the spectrum a peridoc potential in a crystal

IV. Back to gauge theory
   Implication for CP violation in the strong interactions

I. 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 $x_4 \to \pm\infty$
$\to$ Construct from pure gauge configurations on these surfaces, with

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

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

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

Boundary conditions fixed by prevacua: $\begin{array}{r} n_{-\infty} \to |n\rangle \\ n_\infty \to \langle n| \end{array}$ (field eigenstates)

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

Ground state $|\mathrm{vac}\rangle = \mathrm{e}^{-HT} \sum_n \mathrm{e}^{-\mathrm{i}n\theta} |n\rangle$, $\boldsymbol{T} \to \infty$

[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 $T \to \infty$ in the path integral to project on the ground state
- 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 (1976)]
Without ado, this contradicts one of the postulates of quantum theory.
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

II. 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:

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

These commutators hold for (α arbitrary) $\vec{\Pi}^a = \dfrac{\delta}{\mathrm{i}\delta\vec{A}^a} + \alpha\dfrac{g}{8\pi^2}\vec{B}^a\,.$

Hamiltonian density:

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

[Jackiw (1980)]

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

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

States with this property constitute subspaces invariant under the action of the Hamiltonian, i.e. θ' is protected by a superselection rule.
(NB: θ' is independent of θ in the Lagrangian and α in the canonical momentum)

Abstract formulation

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

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

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

Eigensystem of $G(T)$:

$$\Psi_\theta(T\vec{V}) = \mathrm{e}^{\mathrm{i}\theta}\Psi_\theta(\vec{V}) \;\Rightarrow$$

$$\Psi_\theta(T^n\vec{V}) = G^n(T)\Psi_\theta(\vec{V}) = \mathrm{e}^{\mathrm{i}n\theta}\Psi_\theta(\vec{V}) \quad \text{for integer } n$$

(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 $N(T\vec{V}) = N(\vec{V}) + 1$

$$\longrightarrow \Psi_\theta(\vec{V}) = \psi_\theta(\vec{V})\mathrm{e}^{\mathrm{i}N(\vec{V})\theta}$$

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

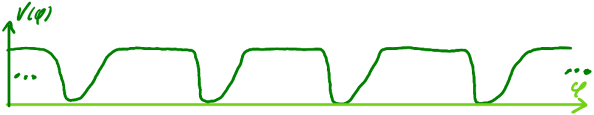
where ψ_θ is periodic in T:

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

Crystal or circle?

The functionals $\Psi(\vec{V})$ with these 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 $\varphi \to \varphi + 2\pi n$ on a circle

On a crystal: Bloch states do not correpsond 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*:

$$\int\limits_{0\leq N(\vec{V})<1} \mathrm{d}\vec{V}\, \Psi^*(\vec{V})\Psi(\vec{V}) = 1\,, \qquad \langle \mathcal{O} \rangle = \int\limits_{0\leq N(\vec{V})<1} \mathrm{d}\vec{V}\, \Psi^*(\vec{V})\mathcal{O}\Psi(\vec{V})$$

III. 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 φ, 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 θ term

Canonical momentum: $\pi_\varphi = \dfrac{\partial L}{\partial \dot{\varphi}} = mR^2(\dot{\varphi} + \omega)$

Hamiltonian: $H = \pi_\varphi \dot{\varphi} - L = \dfrac{1}{2}\dfrac{1}{mR^2}\left(\pi_\varphi - mR^2\omega\right)^2 - \dfrac{1}{2} mR^2\omega^2 + \mathcal{V}(\varphi)$

Momentum operator: $[\varphi, \pi_\varphi] = \mathrm{i} \;\Rightarrow \pi_\varphi = -\mathrm{i}\partial_\varphi - mR^2\omega_B$

Potential at rest and moving

Hamilton operator (ω_B absorbed in ω, constant terms dropped):

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

For $\omega = 0$, standard case of circle with a potential at rest:

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

Time independent Schrödinger equation:

$$\left[\frac{1}{2}\frac{1}{mR^2}\left(\frac{1}{\mathrm{i}}\partial_\varphi\right)^2 + \mathcal{V}(\varphi)\right]\psi(\varphi) = E\psi(\varphi)$$

For potential moving at constant $\omega_\mathcal{V}$, this leads to stationary solutions

$$\left[\frac{1}{2}\frac{1}{mR^2}\left(\frac{1}{\mathrm{i}}\partial_\varphi\right)^2 + \mathcal{V}(\varphi + \omega_\mathcal{V} t)\right]\psi(\varphi + \omega_\mathcal{V} t) = E\psi(\varphi + \omega_\mathcal{V} t)$$

Galilei transformation on a circle

Unitary operator for boosts

$$G(\omega) = \mathrm{e}^{\mathrm{i}\omega N} \text{ where } N = \pi t - mR^2\varphi$$

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

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

$$G(\omega)\psi(\varphi) = \mathrm{e}^{-\mathrm{i}mR^2\omega\varphi}\mathrm{e}^{-\mathrm{i}\frac{mR^2\omega^2 t}{2}}\psi(\varphi + \omega t)$$

Transformation of the previous solution for $\omega_{\mathcal{V}} \neq 0$:

$$G(-\omega_{\mathcal{V}})\psi(\varphi + \omega_{\mathcal{V}} t) = \mathrm{e}^{\mathrm{i}mR^2\omega_{\mathcal{V}}\varphi}\mathrm{e}^{-\mathrm{i}\frac{mR^2\omega_{\mathcal{V}}^2 t}{2}}\psi(\varphi) =: \mathrm{e}^{-\mathrm{i}\frac{mR^2\omega_{\mathcal{V}}^2 t}{2}}\psi'(\varphi)$$

This solves the Schrödinger equation

$$\left[\frac{1}{2}\frac{1}{mR^2}\left(\frac{1}{\mathrm{i}}\partial_\varphi - mR^2\omega_{\mathcal{V}}\right)^2 + \mathcal{V}(\varphi)\right]\psi'(\varphi) = E\psi'(\varphi)$$

$\longrightarrow$ Intuitive interpretation of $\omega_{\mathcal{V}}$/ or θ term

Periodicity condition

Hamiltonian

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

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 $\psi(\varphi) = \mathrm{e}^{-2\pi \mathrm{i} n m R^2 \omega_\theta}\psi(\varphi + 2\pi n)$
- Invariance of QM expectation values under $\varphi \to \varphi + 2\pi n$ likewise only requires periodicity up to a phase

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 $\mathcal{O}(\exp(\mathrm{i}\varphi))$:

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

$\longrightarrow$

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

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

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

$\longrightarrow$

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

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

Consistent time evolution

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

$$\left[H, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right] \ldots \frac{\mathrm{d}}{\ldots}\mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right) \ldots \frac{1}{\ldots}\left[\left(\frac{1}{\ldots}\frac{\partial}{\ldots} + mR^2\omega\right)^2, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right]$$

$$\ldots nR^2\omega\Big)$$

Eigensystem of Hamiltonian:

- For $\omega = 0$ in $H \Rightarrow \psi(\varphi) = \psi(\varphi + 2\pi n)$
- For $\omega \neq 0$ in $H \Rightarrow \psi(\varphi) = \mathrm{e}^{2\pi \mathrm{i} n m R^2 \omega}\psi(\varphi + 2\pi n)$ so that the ω-phases compensate

$\longrightarrow$

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

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

$$0 = \left\langle \mathrm{d}/\mathrm{d}t\, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right\rangle = \int_{0\le\varphi<2\pi} \mathrm{d}\varphi\, \psi^*(\varphi)\left(\mathrm{d}/\mathrm{d}t\, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right)\psi(\varphi)$$

$\longrightarrow$

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

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

Consistent time evolution

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

$$\left[H, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right] = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right) = \frac{1}{2}\left[\left(\frac{1}{\mathrm{i}}\frac{\partial}{\partial\varphi} + mR^2\omega\right)^2, \mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right]$$

$$= -\frac{1}{2}\left(\frac{\partial^2}{\partial\varphi^2}\mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right) - \left(\frac{\partial}{\partial\varphi}\mathcal{O}\left(\mathrm{e}^{\mathrm{i}\varphi}\right)\right)\left(\frac{\partial}{\partial\varphi} + \mathrm{i}mR^2\omega\right)$$

$\longrightarrow$

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

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

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

$\longrightarrow$

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

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

Physics picture

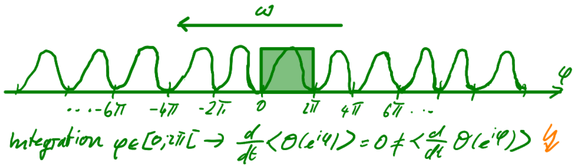
Take $H = -\frac{1}{2}\frac{1}{mR^2}\partial_\varphi^2 + \mathcal{V}(\varphi)$ ($\omega = 0$ can always be achieved by boosts)

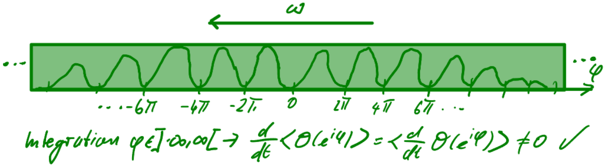
$\psi(\varphi) = \mathrm{e}^{2\pi i n m R^2 \omega}\psi(\varphi + 2\pi n) \longrightarrow$ wave with crystal momentum $\propto \omega$

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





IV. Back to gauge theory

For the Hamiltonian

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

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

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

$$\begin{aligned} K(\vec{A}^a) =& \frac{1}{8\pi^2}\,\epsilon^{ijk}\int \mathrm{d}^3x\left(\frac{1}{2}\,A^{a,i}\partial_j A^{a,k} - \frac{1}{6}\,f^{abc}A^{a,i}A^{b,j}A^{c,k}\right) \\ \Psi'(\vec{A}^a) =& \mathrm{e}^{\mathrm{i}\theta K(\vec{A}^a)}\Psi(\vec{A}^a) \;\Rightarrow\; \mathcal{G}_n\Psi' = \Psi' \\ \mathcal{H}' =& \mathrm{e}^{\mathrm{i}\theta K(\vec{A}^a)}\mathcal{H}\mathrm{e}^{-\mathrm{i}\theta K(\vec{A}^a)} = \frac{1}{2}\left(-g^2\frac{\delta^2}{\delta\vec{A}^{a\,2}} + (\vec{B}^a)^2\right) \end{aligned}$$

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.

THANK YOU!

V. Finite sub(volumes)

Boundary conditions at infinity crucial for alignement 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, Δn is topologically conserved.

Lattice simulations sample over Δn 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 Ω, interfere different topological sectors Δn: [Weinberg QFT]

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

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

(Assume $\Delta n(\Omega) = \Delta n_1(\Omega_1) + \Delta n_2(\Omega_2)$)

$$\langle\mathcal{O}_1\rangle_\Omega = \lim_{\substack{N_2\to\infty \\ N_2\in\mathbb{N}}} \lim_{\substack{N_1\to\infty \\ N_1\in\mathbb{N}}} \frac{\sum_{\Delta n_1=-N_1}^{N_1} \sum_{\Delta n_2=-N_2}^{N_2} f(\Delta n_1+\Delta n_2) \int_{\Delta n_1} \mathcal{D}\phi\, \mathcal{O}_1\, \mathrm{e}^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2} \mathcal{D}\phi\, \mathrm{e}^{-S_{\Omega_2}[\phi]}}{\sum_{\Delta n_1=-N_1}^{N_1} \sum_{\Delta n_2=-N_2}^{N_2} f(\Delta n_1+\Delta n_2) \int_{\Delta n_1} \mathcal{D}\phi\, \mathrm{e}^{-S_{\Omega_1}[\phi]} \int_{\Delta n_2} \mathcal{D}\phi\, \mathrm{e}^{-S_{\Omega_2}[\phi]}}$$

Independence of $\langle\mathcal{O}_1\rangle_\Omega$ from the fluctuations in Ω_2 is achieved if the contributions from Ω_2 cancel (absorb determinant phases in f):

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

Now keep Δn fixed, Ω_2 either finite or infinite:

$$\langle \mathcal{O}_1 \rangle_\Omega = \frac{\sum\limits_{\Delta n_1 = -\infty}^{\infty} f(\Delta n) \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathcal{O}_1 \, \mathrm{e}^{-S_{\Omega_1}[\phi]} \int\limits_{\Delta n_2 = \Delta n - \Delta n_1} \mathcal{D}\phi \, \mathrm{e}^{-S_{\Omega_2}[\phi]}}{\sum\limits_{\Delta n_1 = -\infty}^{\infty} f(\Delta n) \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathrm{e}^{-S_{\Omega_1}[\phi]} \int\limits_{\Delta n_2 = \Delta n - \Delta n_1} \mathcal{D}\phi \, \mathrm{e}^{-S_{\Omega_2}[\phi]}}$$

$$= \frac{\sum\limits_{\Delta n_1 = -\infty}^{\infty} f(\Delta n) I_{\Delta n - \Delta n_1}(2\mathrm{i}\kappa\Omega_2) \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathcal{O}_1 \, \mathrm{e}^{-S_{\Omega_1}[\phi]}}{\sum\limits_{\Delta n_1 = -\infty}^{\infty} f(\Delta n) I_{\Delta n - \Delta n_1}(2\mathrm{i}\kappa\Omega_2) \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathrm{e}^{-S_{\Omega_1}[\phi]}}$$

$$\underset{\Omega_2 \gg \Omega_1}{\approx} \frac{\sum\limits_{\Delta n_1 = -\infty}^{\infty} \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathcal{O}_1 \, \mathrm{e}^{-S_{\Omega_1}[\phi]}}{\sum\limits_{\Delta n_1 = -\infty}^{\infty} \int\limits_{\Delta n_1} \mathcal{D}\phi \, \mathrm{e}^{-S_{\Omega_1}[\phi]}}$$

Corresponds to finite VT, $\theta = 0$

Result also holds for $\Omega_2 \to \infty$, Δn free

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

The theory with fixed Δn (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 $\Omega_2 \to \infty$, the result does not depend on whether Δn is fixed or free.