Topological Structure of the QCD Vacuum

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Therefore, the topological excitations, such as the instantons, plays a central role in understanding the vacuum of QCD.

Since the topological excitations do not occur in the perturbation theory, theoretical calculations starting from the QCD Lagrangian necessarily involves non-perturbative methods, such as lattice QCD.
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(ii) Unquenched simulations with Wilson/staggered fermion do not respect correct chiral or flavor symmetry at finite lattice spacing, and the definition of the topological charge through the Atiyah-Singer index theorem is ambiguous.

(iii) With the HMC algorithm which is based on a continuous evolution of the gauge links, the system is trapped in a fixed topological sector as the continuum limit is approached. Therefore, a proper sampling of different topological sectors cannot be achieved. (Approaching the chiral limit, the suppression of the fermion determinant for $Q \neq 0$ also makes the tunneling a rare event.)
During the last decade, (i) and (ii) have been solved by the realization of exact chiral symmetry on the lattice, with which the topological charge is uniquely defined at any finite lattice spacing by counting the number of fermionic zero-modes.
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However, (iii) remains insurmountable, since the correct sampling of topology becomes increasingly more difficult towards realistic simulation with lighter quarks and finer lattices.

A plausible solution is to perform QCD simulations in a fixed topological sector and to extract topological susceptibility from local topological fluctuations. Then any observable measured at a fixed topological charge can be transcribed to its value in the $\theta$ vacuum.
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Simulations are performed on a $16^3 \times 32$ lattice at lattice spacing $\sim 0.12$ fm at six sea quark masses $m_q$ ranging in $m_s/6 - m_s$. 
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The $\chi_t$ (topological susceptibility) is extracted from the constant behavior of the time-correlation of flavor-singlet pseudo-scalar meson two-point function at large distances, which arises from the finite size effect due to the fixed topology.
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In the small $m_q$ regime, our result of $\chi_t$ is proportional to $m_q$ as expected from chiral effective theory. Using the formula $\chi_t = m_q \Sigma / N_f$ by Leutwyler-Smilga, we obtain $\Sigma^{\overline{MS}}(2$ GeV$) = [252(5)(10)$ MeV$]^3$
Outline

- Introduction
- Topology with Overlap Dirac Operator
- Lattice Setup
- Results using $N_f = 2$ Dynamical Overlap Configurations with $Q_t = 0, -2, -4$
- Conclusion and Outlook
Theoretically, topological susceptibility is defined as

$$
\chi_t = \int d^4 x \langle \rho(x) \rho(0) \rangle
$$

where

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\rho(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)]
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**Veneziano-Witten relation**

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Leutwyler-Smilga relation

\[ \chi_t = \frac{m_q \Sigma}{N_f} + \mathcal{O}(m_q^2) \quad \text{(in the chiral limit)} \]
For lattice QCD with fixed topology in a finite volume, $\chi_t$ is the most crucial quantity which is used to relate any observable measured in the fixed topology to its physical value.

Brower, Chandrasekaran, Negele, Wiese, PLB 560 (2003) 64

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In other words, the artifacts due to fixed topology can be removed, provided that $\chi_t$ has been determined.
Since

$$\chi_t = \int d^4x \langle \rho(x)\rho(0) \rangle = \frac{1}{\Omega} \langle Q_t^2 \rangle, \quad \Omega = \text{volume}$$

where

$$Q_t = \int d^4x \frac{1}{32\pi^2} \epsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)] = \text{integer}$$

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one can obtain \( \chi_t \) by counting the number of gauge configurations for each topological sector.

However, for a set of gauge configurations in the topologically-trivial sector, \( Q_t = 0 \), it gives \( \chi_t = 0 \).
Even for a topologically-trivial gauge configuration, it may possess near-zero modes due to excitation of instanton and anti-instanton pairs, which are the origin of spontaneous chiral symmetry breaking in the infinite volume limit.
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Thus, one can investigate whether there are topological excitations within any sub-volumes, and to measure the topological susceptibility using the correlation of the topological charges of two sub-volumes.
For any topological sector with $Q_t$, using $\chi_{PT}$, it can be shown that

$$\lim_{|x-y| \to \infty} \langle \rho(x) \rho(y) \rangle = \frac{1}{\Omega} \left( \frac{Q_t^2}{\Omega} - \chi_t - \frac{c_4}{2\chi_t\Omega} \right) + \mathcal{O}(\Omega^{-3})$$

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Thus, in the trivial sector with $Q_t = 0$, for any two widely separated sub-volumes $\Omega_1$ and $\Omega_2$, the correlation of their topological charges would behave as

$$\langle Q_1 Q_2 \rangle \simeq -\frac{\Omega_1 \Omega_2}{\Omega} \left( \chi_t + \frac{c_4}{2\chi_t \Omega} \right)$$

$$Q_i = \int_{\Omega_i} d^4x \rho(x)$$
On a finite lattice, consider two spatial sub-volumes at time slices $t_1$ and $t_2$, measure the time-correlation function

$$C(t_1 - t_2) = \langle Q(t_1)Q(t_2) \rangle = \sum_{\vec{x}_1, \vec{x}_2} \langle \rho(x_1)\rho(x_2) \rangle$$
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Then its plateau at large $|t_1 - t_2|$ can be used to extract $\chi_t$ provided that

$$|c_4| \ll 2\chi_t^2\Omega, \quad c_4 = -\frac{1}{\Omega} \left[ \langle Q_t^4 \rangle_{\theta=0} - 3\langle Q_t^2 \rangle_{\theta=0}^2 \right]$$
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However, on a lattice, it is difficult to extract $\rho(x)$ unambiguously from the link variables!
It is well known that the topological charge density can be defined via the overlap Dirac operator as

$$\rho(x) = \text{tr}[\gamma_5(1 - rD)_{x,x}], \quad r = \frac{1}{2m_0}$$

where $D$ is the overlap Dirac operator

$$D = m_0(1 + V), \quad V = \gamma_5 \frac{H_w}{\sqrt{H_w^2}},$$

$$H_w = \gamma_5(-m_0 + \gamma_\mu t_\mu + W)$$
Here $\rho(x) = \text{tr} [\gamma_5 (1 - rD)_{x \neq x}]$ is justified to be a definition of topological charge density since it has been asserted (Kikukawa & Yamada, 1998)

$$\rho(x) \xrightarrow{a \to 0} \frac{1}{32\pi^2} \epsilon_{\mu\nu\lambda\sigma} \text{tr} [F_{\mu\nu}(x) F_{\lambda\sigma}(x)]$$
Topology with Overlap Dirac Operator (cont)

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\rho(x) \xrightarrow{a \to 0} \frac{1}{32\pi^2} \varepsilon_{\mu\nu\lambda\sigma} \text{tr}[F_{\mu\nu}(x)F_{\lambda\sigma}(x)]
\]

Note that the index theorem on the lattice

\[
\text{index}(D) = n_+ - n_- = \sum_x \rho(x) = Q_t
\]

had been observed by Narayanan and Neuberger in 1995, using the spectral flow of \( H_w(m_0) \), before the Ginsparg-Wilson relation was rejuvenated in 1998.
It seems natural to use $\rho(x) = \text{tr}[\gamma_5 (1 - rD)_{x,x}]$ to compute the topological susceptibility

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\chi_t = \frac{1}{\Omega} \langle Q_t^2 \rangle = \frac{1}{\Omega} \sum_{x,y} \langle \rho(x) \rho(y) \rangle = \sum_x \langle \rho(x) \rho(0) \rangle
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\]

On the other hand, one can derive the relation

\[
\text{index}(D) = m \sum_x \text{tr}\left[\gamma_5(D_c + m)^{-1}_{x,x}\right] = m \text{ Tr}\left[\gamma_5(D_c + m)^{-1}\right]
\]

where

\[
D_c = D(1 - rD)^{-1} = 2m_0(1 + V)(1 - V)^{-1}
\]

is chirally symmetric but non-local (Chiu & Zenkin, 1998). Note that for the topologically-trivial configurations, \( D_c \) is well-defined (without any poles).
Thus one can regard

\[ \rho_1(x) = m \, \text{tr}[\gamma_5(D_c + m)^{-1}]_{x,x} \]

as a definition of topological charge density, for any valence quark mass \( m \).
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Obviously, the identity \( \text{index}(D) = m \, \text{Tr} \left[ \gamma_5 (D_c + m)^{-1} \right] \) can be generalized to
\[ \text{index}(D) = m_1 m_2 \cdots m_k \text{Tr} \left[ \gamma_5 (D_c + m_1)^{-1} (D_c + m_2)^{-1} \cdots (D_c + m_k)^{-1} \right] \]
with the generalized topological charge density
\[ \rho_k(x) = m_1 m_2 \cdots m_k \text{tr} \left[ \gamma_5 (D_c + m_1)^{-1} (D_c + m_2)^{-1} \cdots (D_c + m_k)^{-1} \right] \]
Presumably, any $\rho_k$ can be used to compute $\chi_t$. In general,

$$\chi_t = \frac{m_1 \cdots m_km_{k+1} \cdots m_l}{\Omega} \langle \text{Tr}[\gamma_5(D_c + m_1)^{-1} \cdots (D_c + m_k)^{-1}] \times \text{Tr}[\gamma_5(D_c + m_{k+1})^{-1} \cdots (D_c + m_l)^{-1}] \rangle$$
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$$

It has been pointed out by Lüscher, for $k \geq 2$ and $l \geq 5$, $\chi_t$ avoids the short-distance singularities in the continuum limit.
However, on a finite lattice,

\[
\lim_{|x-y| \gg 1} \langle \rho_1(x) \rho_1(y) \rangle \simeq \frac{1}{\Omega} \left( \frac{Q_t^2}{\Omega} - \chi t - \frac{c_4}{2 \chi t \Omega} \right) + O(e^{-m_\pi |x-y|}) + O(e^{-m_{\eta'} |x-y|}) + O(\Omega^{-3}) + \ldots
\]

is contaminated by \( m_\pi, m_{\eta'}, \ldots \), which can couple to \( \langle \rho_1(x) \rho_1(y) \rangle \).
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$$+ O\left(e^{-m_{\eta'} |x-y|}\right) + O\left(\Omega^{-3}\right) + \cdots$$

is contaminated by $m_\pi, m_{\eta'}, \cdots$, which can couple to $\langle \rho_1(x) \rho_1(y) \rangle$.

A better alternative is to compute the correlator of flavor-singlet $\eta'$, which behaves as

$$\lim_{|x-y| \gg 1} m_q^2 \langle \eta'(x) \eta'(y) \rangle \simeq \frac{1}{\Omega} \left( \frac{Q_t^2}{\Omega} - \chi_t - \frac{c_4}{2 \chi_t \Omega} \right) + O\left(e^{-m_{\eta'} |x-y|}\right)$$

$$+ O\left(\Omega^{-3}\right) + \cdots$$

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Time-Correlation Function of $\eta'$

$$C_{\eta'}(t) = \frac{1}{N_r} \sum_{\rightarrow x} \times$$

$$- \sum_{\rightarrow x} \times$$
Lattice Setup

- Lattice size: $16^3 \times 32$
- Gluons: Iwasaki gauge action at $\beta = 2.30$
- Quarks ($N_f = 2$): overlap Dirac operator with $m_0 = 1.6$
- Add extra Wilson fermions and pseudofermions

$$\text{det}(H_{ov}^2) \longrightarrow \text{det}(H_{ov}^2) \frac{\text{det}(H_{w}^2)}{\text{det}(H_{w}^2 + \mu^2)}, \quad \mu = 0.2$$

This forbids $\lambda(H_w)$ crossing zero, thus $Q_t$ is invariant.

- Quark masses: $m_{sea} = 0.015, 0.025, 0.035, 0.050, 0.070, 0.100$, each of 500 confs with $Q_t = 0$. For $m_{sea} = 0.05$, 250 confs with $Q_t = -2, -4$ respectively.

- For each configuration, 50 conjugate pairs of low-lying eigenmodes of overlap Dirac operator are projected.
$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$

no. of confs = 520

disconnected (hairpin)
$C(t)$

- $16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$
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Disconnected (hairpin) and connected states.
$16^3 \times 32, \beta = 2.30, m_{\text{sea}} = m_{\text{val}} = 0.025$

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- $\eta' = \text{hairpin - connected} / N_f$

Diagram shows $C(t)$ vs $t$ with data points indicating disconnected (hairpin) and connected states.
$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$

no. of confs = 520

- disconnected (hairpin)
- connected

$-\eta' = \text{hairpin} - \text{connected} / N_f$

cosh + $c_{\eta'}$
$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$

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$C(t)$

t
Saturation of $\eta'$ by low-lying eigenmodes

$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$

no. of configurations = 520

$-C_{\eta}'(t)$

nev = 10 + 10
Saturation of $\eta'$ by low-lying eigenmodes

$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.025$

no. of configurations = 520

- $nvt = 10 + 10$
- $nvt = 20 + 20$
Saturation of $\eta'$ by low-lying eigenmodes

$16^3 \times 32$, $\beta=2.30$, $m_{\text{sea}}=m_{\text{val}}=0.025$

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no. of configurations = 520

$-C_{\eta}(t)$

- $\circ$ nev = 10 + 10
- $\diamond$ nev = 20 + 20
- $\square$ nev = 30 + 30
- $\star$ nev = 40 + 40
- $\triangle$ nev = 50 + 50

$0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30$

$-5.0 \times 10^{-3} \quad -4.0 \times 10^{-3} \quad -3.0 \times 10^{-3} \quad -2.0 \times 10^{-3} \quad -1.0 \times 10^{-3} \quad 0.0$
Realization of Leutwyler-Smilga relation

In the limit $m \to 0$, $\chi_t \to m\Sigma/N_f$, in agreement with ChPT.

$\Sigma^{MS}(2 \text{ GeV}) = [252(5)(6) \text{ MeV}]^3$

ChPT $\chi_t = m\Sigma/n_f$
Determination of $\Sigma$

From the slope of the linear fit of $\chi_t$ vs. $m_q$ for $m_q a = 0.015, 0.025$, and $0.035$, it gives

$$a^3 \Sigma = 0.00257(10)$$

With $a^{-1} = 1670(20)(20)$ MeV, and $Z_{m}^{\overline{MS}}(2 \text{ GeV}) = 0.742(12)$, the value of $a^3 \Sigma$ is transcribed to

$$\Sigma^{\overline{MS}}(2 \text{ GeV}) = (252 \pm 5 \pm 10 \text{ MeV})^3$$

in good agreement with our previous result $251(7)(11)$ MeV obtained in the $\epsilon$-regime.

Universality of $\chi_t$ for different Topological Sectors

$16^3 \times 32$, $\beta = 2.30$, $m_{\text{sea}} = m_{\text{val}} = 0.050$

- $Q_t = 0$, 500 confs.
- $Q_t = -2$, 250 confs.
- $Q_t = -4$, 250 confs.
For the topologically-trivial gauge configurations generated with $N_f = 2$ dynamical overlap quarks constrained by extra Wilson and pseudofermions, they possess topologically non-trivial excitations (e.g., instanton and anti-instanton pairs) in sub-volumes.
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These near-zero modes allow us to determine $\chi_t$ and $\Sigma$. 
Conclusion and Outlook

- For the topologically-trivial gauge configurations generated with $N_f = 2$ dynamical overlap quarks constrained by extra Wilson and pseudofermions, they possess topologically non-trivial excitations (e.g., instanton and anti-instanton pairs) in sub-volumes.

- These near-zero modes allow us to determine $\chi_t$ and $\Sigma$.

- In the chiral limit, $\chi_t = m\Sigma/N_f$ is realized, with $\Sigma^{\overline{MS}}(2 \text{ GeV}) = 252(5)(10)$ MeV, in good agreement with our result in $\epsilon$-regime.
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For $m_{sea} = 0.05$, $\chi_t$ extracted from different topological sectors ($Q_t = 0, -2, -4$) are consistent with each other.
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It remains to obtain an upper bound of $c_4$ (from 2-pt and 4-pt correl. fn.) to see whether $|c_4| \ll 2\chi_t^2\Omega$ is satisfied.