CHAPTER 6

Topology with Wilson fermions

One of the most intriguing features of QCD is its topological vacuum structure which has phenomenological consequence related to $\eta'$ mass given by Witten and Veneziano formula [80] (which is derived in the limit of large number colors) connecting the mass of the $\eta'$ meson to the quenched topological susceptibility ($\chi^{qu}$) of QCD. This formula takes its simplest form in the chiral limit:

$$m_{\eta'}^2 = \frac{2N_c}{F_{\pi}^2} \chi^{qu}$$

The topological charge fluctuations in QCD vacuum are characterized by the topological susceptibility ($\chi$). Since the topological excitations do not occur in the perturbation theory, calculation of $\chi$ needs non-perturbative technique.

In this chapter we first describe some topological properties of QCD vacuum in continuum and then we describe how far those can be reproduced in simulation with unimproved Wilson fermion and Wilson gauge action in lattice.

6.1 Topological charge and susceptibility in continuum

We start with the flavour singlet axial Ward identity given by,

$$\langle \partial_{\mu} J_{\mu} (x) \rangle = 2m \langle \bar{\psi}(x) \gamma_{5} \psi(x) \rangle - 2q(x) \tag{6.1}$$

where $q(x) = \frac{g^2}{32\pi} \varepsilon_{\mu\nu\rho\lambda} \text{tr}_{C} \left( F_{\mu\nu}(x) F_{\rho\lambda}(x) \right)$ is topological charge density and topological charge ($Q$) is defined as $Q = \int d^4x \ q(x)$. Note that in the flavour singlet axial Ward identity given by Eq. (6.1) is true for any background gauge fields which means integrations only over the fermion fields are performed.
6.1.1 Index theorem

Index theorem connects topological charge with the zero modes of Dirac operator. Following Ref. [81] here we give a heuristic derivation of this theorem in continuum. Integrating both sides of Eq. (6.1) over Euclidean four volume, left hand side vanishes and we get

\[ Q = \int d^4 x \, m(\overline{\psi}(x) \gamma_5 \gamma_5 \psi(x)) \]
\[ = m \, \text{tr} \left( \gamma_5 G \right) \]
\[ = m \, \text{tr} \left( \frac{1}{i\gamma_5 + m} \right) \]
\[ = m \sum_s \frac{f_s^\dagger \gamma_5 f_s}{i\lambda_s + m}, \quad \lambda_s \in \mathbb{R}. \quad (6.2) \]

where \( f_x \) are the eigenfunctions of the (antihermitian) Dirac operator \( \gamma \) with eigenvalues \( i\lambda_s \),

\[ \gamma f_s = i\lambda_s f_s, \quad \lambda_s \in \mathbb{R}. \quad (6.3) \]

We choose orthonormalised eigenvectors such that

\[ f_s^\dagger f_t = \delta_{st}. \quad (6.4) \]

The chirality of an eigenvector is given by \( f_s^\dagger \gamma_5 f_s \). Now since the Dirac operator anti commutes with \( \gamma_5 \) the spectrum is symmetric about zero:

\[ \text{sp}(\gamma) = \{\pm i\lambda_s, \lambda_s \in \mathbb{R} \} \quad (6.5) \]

where for \( \lambda_s \neq 0 \), \( \gamma_5 f_s \) is also an eigenfunction with eigenvalue \( -i\lambda_s \) and chirality = 0. The zero modes, \( \lambda_s = 0 \) can be chosen with definite chirality = ±1. Hence from Eq. (6.2) the right hand side contributes only for zero modes and gives,

\[ Q = n_+ - n_- \quad (6.6) \]

where \( n_+ \) and \( n_- \) are number of zero modes with positive and negative chiralities respectively. Hence because of the Index theorem \( Q \) is expected to be an integer.

6.1.2 Topological susceptibility: chiral behaviour

The topological susceptibility \( \chi \) is defined as the mean squared charge per unit volume,

\[ \chi = (Q^2)/V. \quad (6.7) \]
Another expression of $\chi$ in terms of topological charge density is as follows,

$$\chi = \int d^4x(q(x)q(0)).$$  

(6.8)

Using translational invariance of vacuum it can be easily shown that the above two expressions for $\chi$ are equivalent.

An easy way to see the effect of vanishing quark mass on $\chi$ is by looking at the dependence of fermion determinant on $Q$. Let us separate the contributions to the fermion determinant by zero and nonzero modes for a given gauge-field configuration. For $N_f$ degenerate flavours we have ([80], [82], [83])

$$\prod_{f=1}^{N_f} \det(\not{D} + m) = \prod_{f=1}^{N_f} \left[ m^{n^+ + n^-} \prod_{n,\lambda_n > 0} \left( \lambda_n^2 + m^2 \right) \right]$$  

(6.9)

Hence the gauge configurations with nontrivial topology tend to be suppressed as $m \rightarrow 0$ and in chiral limit only the gauge configurations with $n^+ = n^- = 0 \Rightarrow Q = 0$ will contribute. This means $\chi$ vanishes in the chiral limit.

We can obtain the analytic form of the quark mass dependence of $\chi$ in chiral regime using Ward-Takahashi identity. Now let us consider the flavour singlet axial transformation:

$$\delta\psi = i\alpha_A \frac{1}{2} \gamma_5 \psi \text{ and } \delta\overline{\psi} = i\overline{\psi} \alpha_A \frac{1}{2} \gamma_5.$$

Then for a general operator $\mathcal{O}(y)$, using Eq. (5.25) we get the flavour singlet axial WTI,

$$\partial_\mu \langle A^0_\mu(x)\mathcal{O}(y) \rangle = 2m \langle P^0(x)\mathcal{O}(y) \rangle + 2N_f \langle q(x)\mathcal{O}(y) \rangle - \langle \frac{\delta \mathcal{O}(y)}{\delta \alpha_A(x)} \rangle.$$  

(6.10)

Integrating both sides of the above equation over the four volume we get

$$0 = 2m \int d^4x \langle P^0(x)\mathcal{O}(y) \rangle + 2N_f \int d^4x \langle q(x)\mathcal{O}(y) \rangle - \int d^4x \langle \frac{\delta \mathcal{O}(y)}{\delta \alpha_A(x)} \rangle.$$  

(6.11)

In Eq. (6.11) choosing $\mathcal{O}(y) = q(0)$ we get

$$0 = 2m \int d^4x \langle P^0(x)q(0) \rangle + 2N_f \int d^4x \langle q(x)q(0) \rangle.$$  

(6.12)

For $\mathcal{O}(y) = P^0(0)$ Eq. (6.11) reduces to

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0 = 2m \int d^4x (P^0(x)P^0(0)) + 2N_f \int d^4x (q(x)P^0(0)) - 2 \langle S^0(0) \rangle \tag{6.13}

S^0 \equiv \text{scalar density. Putting together Eqs. (6.12 and 6.13) we obtain}

\chi \equiv \int d^4x (q(x)q(0)) = 4m \langle S^0(0) \rangle + 2N_f \langle S^0(0) \rangle - 2 \int d^4x (P^0(x)P^0(0)) \tag{6.14}

Due to the spontaneous chiral symmetry breaking, \langle S^0(0) \rangle is finite in chiral limit. Hence \chi vanishes linearly in the chiral limit.

According to the leading order chiral perturbation theory [82] in the physical regime (x = \(N_f \Sigma V m' >> 1\) where \(m'\) is the reduced mass of the quark flavours)

\chi = N_f \Sigma m'. \tag{6.15}

Thus for large enough volume chiral perturbation theory predicts the suppression of \chi when mass of at least one quark flavour becomes small.

### 6.2 Lattice topological charge density operator

A rather natural and most simple definition of \(q(x)\) on lattice was given by Peskin [84]. This definition is as follows,

\[ q^\rho(n) = -\frac{\epsilon_{\mu\nu\rho\sigma}}{32\pi^2} tr[U_{\mu
u}U_{\nu\rho}U_{\rho\sigma}] \tag{6.16} \]
where

$$U_{\mu \nu} = U_{\mu \nu} U_{\mu+\nu, \nu} U_{\mu+\nu, \nu}^\dagger U_{\mu, \nu}^\dagger \equiv \exp \{ i \sum \mathcal{F}_{\mu \nu}^b T^b \}. \quad (6.17)$$

It can be easily shown,

$$\mathcal{F}_{\mu \nu}^b \xrightarrow{a \to 0} g a^2 F_{\mu \nu}^b(x_n) + \mathcal{O}(a^3). \quad (6.18)$$

From Eqs. (6.16), (6.17) and (6.18) it immediately follows,

$$q^p(n) \xrightarrow{a \to 0} a^4 q(x_n) + \mathcal{O}(a^5) \quad (6.19)$$

We see that $q^p$ is a sum of eight-link Wilson loops. Moreover, because of the $\varepsilon_{\mu \nu \rho \sigma}$ tensor, $q^p$ contains links in every one of the four space-time directions. But this definition does not symmetrically treat the positive and negative directions of each axis and this prevents $q^p$ from having definite parity. The problem is easily overcome by the symmetrized definition [85] (Fig. 6.2)

$$q(n) \equiv -\frac{1}{2^4 32 \pi^2} \sum_{(\mu, \nu, \rho, \sigma) = \pm 1} \varepsilon_{\mu \nu \rho \sigma} \operatorname{tr}[U_{\mu \nu} U_{\rho \sigma}] \quad (6.20)$$

where, $1 = \varepsilon_{1234} = -\varepsilon_{-1234}$.

There are other improved construction for lattice topological charge density operator.

5Li: The five-loop improved operator of de Forcrand, Perez, and Stamatescu [86, 87], built from a linear combination of five operators in the form of the twisted plaquette, but with the plaquettes replaced by various $m \times n$ rectangular Wilson loops.

Boulder: The lattice approximation developed for SU(2) by DeGrand, Hasenfratz and Kovacs [88], modified for SU(3) by Hasenfratz and Nieter [89] and implemented in the MILC code [67]. It involves a combination of two contorted Wilson loop operators in the fundamental and adjoint representations of SU(3), both defined on closed ten-link paths described by unit lattice vector displacements in the sequence $\{x,y,z,-y,-x,t,x,-t,-x,-z\}$ and $\{x,y,z,-x,t,-z,x,-t,-x,-y\}$ plus rotations and cyclic permutations. This operator was optimized to reduce lattice corrections for small instantons with radii close to the lattice spacing $R \approx a$. 

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All these operators are equivalent in the continuum limit, but they are subject to different discretization effects. MILC collaboration has compared different methods for measuring the topological charge on lattice and selected the Boulder method with hypercubic blocking, since it appears best capable of preserving small instantons at lattice spacings 0.12 and 0.09 fm [90]. We also have used the Boulder definition in this work.

6.3 Smearing

Before measurement the original link fields are smeared by applying up to 20 levels of 4D HYP smearing with optimized parameters as stated in previous chapters. Smearing brings the topological charges close to integer values and behaviour is better for the smaller lattice spacing, as expected.

6.4 Results

6.4.1 Integerness of topological charge

Topological charges of unsmeared configurations are not integer. Smearing brings topological charge close to integer. As expected at smaller lattice spacing ($\beta = 5.8$) it takes less smearing than the larger lattice spacing ($\beta = 5.6$).

In Fig. 6.3 we show the behaviour of topological charge of gauge configurations with smear levels for $\beta = 5.6$ (left) and at $\beta = 5.8$ (right). It is evident that for $\beta = 5.8$ the topological charges of different configurations are clustering about the integer values after about 10
smear levels and values are stable under further smear levels whereas at $\beta = 5.6$ it takes almost 20 smear levels. Because of CP symmetry only multiplicative renormalization applies for topological charge. One method as suggested in Ref. [91] to calculate this multiplicative renormalization makes use of the fact that in fine enough lattices the overall distribution of $Q$ tend to cluster around integers. We calculate the average relative deviation of $Q$ from its closest integer for both $\beta$’s and find in both cases (Fig. 6.4) after smear level 10 the average relative deviations are less than $5\%$ and hence this effect is neglected in the following discussions.

### 6.4.2 Trapping

Approach to the continuum and chiral limits may still be hampered by the phenomenon of critical slowing down. One of the manifestation of critical slowing down is the increase in autocorrelation times associated with the measurements of various observables. “As the continuum limit is approached, lattice QCD simulations tend to get trapped in the topological charge sectors of field space and may consequently give biased results in practice” (Luscher and Schaefer [92]). In Fig. 6.5 we show the Monte Carlo time history of topological charge for

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**Figure 6.3:** **Left figure:** Topological charge of gauge configurations versus HYP smear levels for $\beta = 5.6$ and $\kappa = 0.1583$ at lattice volume $32^3 \times 64$. **Right figure:** Topological charge of gauge configurations versus HYP smear levels for $\beta = 5.8$ and $\kappa = 0.15475$ at lattice volume $32^3 \times 64$. 
Figure 6.4: The average relative deviation of $Q$ from its closest integer versus smear levels at $\beta = 5.6$ and 5.8.

Figure 6.5: The Monte Carlo trajectory history for topological charge at smear level 20 with unimproved Wilson fermion and gauge action for (a) $\beta = 5.6$ with a gap of 24 trajectories between two consecutive measurements and (b) $\beta = 5.8$ with a gap of 32 trajectories between two consecutive measurements.
\( \beta = 5.6 \) and 5.8 for the smallest and the largest \( \kappa \) and there is some evidence of trapping of the topological charge only at \( \beta = 5.8 \) and largest \( \kappa \).

6.4.3 Distribution of topological charge

Fig. 6.6 displays six histograms of topological charge distributions, for two values of \( \beta \) and different volumes. The topological charge data were put in several bins and the bin widths were chosen to be unity centered around the integer values of the topological charges for all the cases. From theoretical considerations the distribution of the topological charge is expected to be a Gaussian [93]. Since our configurations are large in number but finite, an incomplete spanning of the topological sectors may occur and \( \langle Q \rangle \) may not be zero. Hence we define the susceptibility to be

\[
\chi = \frac{1}{V} \left( \langle Q^2 \rangle - \langle Q \rangle^2 \right). \tag{6.21}
\]

The expected distribution is

\[
n_Q = \frac{n_{\text{meas}}}{\sqrt{2\pi(\langle Q^2 \rangle - \langle Q \rangle^2)}} \exp \left( -\frac{(Q - \langle Q \rangle)^2}{2(\langle Q^2 \rangle - \langle Q \rangle^2)} \right), \tag{6.22}
\]

where \( n_{\text{meas}} \) is the total number of measurements made. The Gaussian curves in Fig. 6.6 are obtained by using Eq. (6.22). It is evident from Fig. 6.6 that for a given \( \beta \) and volume the width of the distribution decreases as \( \kappa \) increases, indicating that the topological susceptibility \( \chi \) decreases with decreasing quark mass.

6.4.4 Measurement of topological susceptibility

In Fig. 6.7 topological susceptibility is plotted versus smear level at \( \beta = 5.8, \kappa = 0.15462 \) and lattice volume \( 32^3 \times 64 \). Fig. 6.7 shows that \( \chi \) is very stable with the change of smear level after smear level =3. We have taken 20 smear levels for the measurement of \( \chi \). Since our configurations are large in number but finite, an incomplete spanning of the topological sectors may occur and \( \langle Q \rangle \) may not be zero. Hence we define the susceptibility to be

\[
\chi = \frac{1}{V} \left( \langle Q^2 \rangle - \langle Q \rangle^2 \right). \tag{6.23}
\]

In table 6.1 we present our data for \( \chi \) at \( \beta = 5.6 \) and 5.8 for several \( \kappa \)'s.
Figure 6.6: The topological charge distribution for (a) $\beta = 5.6$, $\kappa = 0.15775$, volume $= 16^3 \times 32$
(b) $\beta = 5.6$, $\kappa = 0.15775$, volume $= 24^3 \times 48$ (c) $\beta = 5.6$, $\kappa = 0.15775$, volume $= 32^3 \times 64$
(d) $\beta = 5.6$, $\kappa = 0.15825$, volume $= 24^3 \times 48$ (e) $\beta = 5.8$, $\kappa = 0.1543$, volume $= 32^3 \times 64$ (f) $\beta = 5.8$, $\kappa = 0.15475$, volume $= 32^3 \times 64$. 

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Table 6.1: Dimensionless topological susceptibilities.
To take the effect of the auto-correlations on the error estimate into account, we multiplied the naive errors by $\sqrt{2\tau_{\text{int}}}$. The measurement of the integrated auto-correlation time, however, may not be very accurate due to limited statistics.

### 6.4.5 Chiral behaviour of topological susceptibility

For ease of comparison with earlier presentations of results and clarification we present for $\beta = 5.6$ and 5.8 at lattice volume $32^3 \times 64$, topological susceptibility versus $m_\pi^2$ in the units of $r_0$ (quark mass dependent), (i.e., in mass-dependent renormalization scheme) in Fig. 6.8. At $\beta = 5.6$ our second largest quark mass (in Fig. 6.8) is very close to the lowest quark mass of Ref. [9]. In this figure the shaded region corresponds to $m_\pi \geq 500$ MeV. In the lower pion mass region our data for both $\beta = 5.6$ and 5.8 clearly show the suppression even in mass-dependent renormalization scheme.

Fig. 6.9 shows our results for topological susceptibility versus $m_\pi^2$, in the units of Sommer parameter ($r_0$) at the chiral limit (i.e., in the mass-independent renormalization scheme),
Figure 6.8: Topological susceptibility versus $m^2$ in the units of $r_0$ (quark mass dependent) for $\beta = 5.6$ and 5.8 and at lattice volume $32^3 \times 64$.

Figure 6.9: Topological susceptibility versus $m^2$ in the units of $r_0$ (at chiral limit) for $\beta = 5.6$ and at lattice volumes $16^3 \times 32$, $24^3 \times 48$, and $32^3 \times 64$ compared with the results of SESAM-T\chi L collaborations.
for $\beta = 5.6$ and at lattice volumes $16^3 \times 32$, $24^3 \times 48$, and $32^3 \times 64$. We also show the results of SESAM-T$\chi$L collaborations [9]. Using the numbers given in [9], we have replotted it after scaling by the value of $r_0$ quoted at the physical point. This new plot clearly shows the suppression of susceptibility with decreasing quark mass in the earlier SESAM-T$\chi$L data with unimproved Wilson fermion. Our results carried out at larger volume and smaller quark masses unambiguously (i.e., independent of the renormalization schemes used) establish the suppression of topological susceptibility with decreasing quark mass in accordance with the chiral Ward identity and chiral perturbation theory. Further we note that, for a given $\kappa$, the value of topological susceptibility increases with the volume as expected from finite volume considerations. This effect is more noticeable in smaller volumes. For large enough volume topological susceptibility should be independent of volume, since $(Q^2)$ scales with the volume.

Since unimproved Wilson fermion has $O(a)$ lattice artifacts it is important to estimate the scaling violations of our results. Fig. 6.10 (left) shows topological susceptibility in the physical units for $\beta = 5.6$ and $\beta = 5.8$ at lattice volume $32^3 \times 64$ versus nonperturbatively renormalized [69] quark mass in $\overline{\text{MS}}$ scheme [94] at 2 GeV. Topological susceptibility at $\beta = 5.8$ approximately matches with that at $\beta = 5.6$ within the error bars but the latter data is systematically below the former. This behaviour which is qualitatively consistent with leading order lattice artifact [85] is observed also by the MILC collaboration [95]. For comparison, in Fig. 6.10 (left), we have also shown the results of mixed action calculation of Ref. [96] at $\beta = 5.3$ where the authors have quoted two separate lattice spacings, $a = 0.0784$ fm and $a = 0.070$ fm for the same $\beta$. The calculation of Ref. [96] employs gauge configurations generated with dynamical $O(a)$ improved Wilson fermion, using DD-HMC algorithm and topological charge is measured using a fermionic operator, namely, the Neuberger-Dirac operator.

Fig. 6.10 (left) shows that our results of the topological susceptibility favourably compare with that of Ref. [96].

In Fig. 6.10 (right) we show topological susceptibility in the physical units for $\beta = 5.6$ and $\beta = 5.8$ at lattice volume $32^3 \times 64$ versus nonperturbatively renormalized [69] quark mass in $\overline{\text{MS}}$ scheme [94] at 2 GeV. The leading order chiral perturbation theory prediction, $\chi = \frac{1}{2} \Sigma m_q$ where $\Sigma$ is the chiral condensate, is also shown for the range $230 \text{ MeV} < \Sigma < 290 \text{ MeV}$. The
Figure 6.10: **Top Figure:** Topological susceptibility versus $m_q$ in the physical units for $\beta = 5.6$ and $\beta = 5.8$ at lattice volume $32^3 \times 64$ compared with the results of mixed action (Clover and Overlap). **Bottom Figure:** Topological susceptibility versus $m_q$ in the physical units for $\beta = 5.6$ and $\beta = 5.8$ at lattice volume $32^3 \times 64$ compared with the leading order chiral perturbation theory prediction.
topological susceptibility at $\beta = 5.8$ is consistent with leading order chiral perturbation theory prediction.