

Dirac eigenspectrum and the fate of anomalous U(1) chiral symmetry in thermal QCD

By

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To Nature

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ABSTRACT

This thesis presents a systematic investigation into the thermal phases and properties of strongly interacting nuclear matter described by Quantum Chromodynamics (QCD), focusing on the effective restoration of the different subgroups of the almost exact two-flavor chiral symmetry. From the properties of the eigenvalue spectrum of the quark Dirac operator calculated using lattice techniques, this thesis addresses the specific implications of the effective restoration, specifically of the anomalous singlet subgroup of chiral symmetry. Understanding the fate of chiral symmetry in QCD is of fundamental importance since its breaking is responsible for the origin of more than 99% of the mass of the visible universe.

The first major finding establishes that the anomalous breaking of the singlet $U_A(1)$ symmetry persists well into the high-temperature regime, where the non-singlet chiral symmetry is effectively restored. Through a detailed analysis of the most infrared part of the QCD Dirac spectrum, we show that this non-trivial breaking is driven entirely by a distinct peak-like accumulation of near-zero Dirac eigenmodes. By performing simulations on a very fine lattice, we show that this infrared spectral peak is a genuine physical feature of the thermal QCD vacuum rather than a numerical artifact. We also demonstrate that the non-trivial breaking of $U_A(1)$ due to these infrared eigenvalues gradually gets effectively restored at higher temperatures $\sim 1.2 T_{pc}$, where T_{pc} represents the pseudo-critical temperature corresponding to the effective restoration of the non-singlet subgroup of the two-flavor chiral symmetry. This result is obtained after performing a continuum extrapolation using data from different lattice spacings, and should be independent of specific

lattice discretization for the Dirac operator. We nevertheless check the robustness of our observations using a fermion discretization which preserves the chiral symmetry to a very good extent even on a finite lattice.

However performing lattice QCD calculations using such fermion discretizations comes with formidable computational cost. By implementing high-level optimizations, we significantly increase the efficiency of our algorithm. Furthermore using such fermion discretization allows us to determine the topological fluctuations of the QCD vacuum more accurately even on a finite lattice. We argue that the temperature dependence of topological charge fluctuations can give us indication of the sequential restoration of different subgroups of the two-flavor chiral symmetry in QCD. Whereas the temperature dependence of topological fluctuations agreeing with prediction from a dilute instanton gas model can tell us about effective restoration of $U_A(1)$, its deviation from its value known from chiral perturbation theory can indirectly hint at the restoration of the non-singlet subgroup. Our results clearly supports a sequential hierarchy in the restoration of chiral symmetry.

Furthermore, we demonstrate deep connections between the structural properties of the most infrared Dirac eigenstates and the effective restoration of the different subgroups of chiral symmetry in QCD. Immediately above the pseudo-critical temperature these infrared Dirac eigenstates are delocalized but non-ergodic and are fractal-like, whose fractal dimensions carry information about the universal critical scaling that is otherwise visible in the thermodynamic observables only in the chiral limit. We also propose that the change in curvature of these infrared eigenstates due to a twist applied on one of the spatial boundaries of the lattice, quantified by the Thouless conductance, is a sensitive indicator of the effective restoration of the $U_A(1)$ symmetry. Finally, we show that the not-so infrared bulk eigenmodes in high temperature QCD contain signatures of quantum chaos. Along with the fact that classical states exist which exhibit classical chaos we could demonstrate a non-trivial realization of the Bohigas-Giaconni-Schmidt conjecture in QCD.

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Chapter 1

Introduction

1.1 The QCD phase diagram

The unraveling of the phase diagram of Quantum Chromodynamics (QCD) under extreme conditions due to temperature and net baryon density, or equivalently baryon chemical potential μ_B , represents a frontier in modern nuclear theory research [1, 2]. The different phases of the QCD phase diagram arise from the intricate interplay of two distinct, non-perturbative phenomena inherent to the strong interaction i.e., color confinement and the spontaneous breaking of chiral symmetry. In this thesis, we investigate the thermal restoration of chiral symmetry and explore its microscopic signatures across the QCD phase transition.

The thermodynamics of QCD at finite temperature T is entirely encoded in the grand canonical partition function, $\mathcal{Z} = \text{Tr}[e^{-H_{QCD}/T}]$ which can be equivalently expressed as a Euclidean path integral over the microscopic gauge and fermion degrees of freedom [2, 3],

$$\mathcal{Z}(T, V) = \int \mathcal{D}[A_\mu] \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] \exp\left(-\int_0^{1/T} d\tau \int_V d^3x \mathcal{L}_E\right). \quad (1.1)$$

The statistical weight of each field configuration is determined by the Euclidean action,

given by the spacetime integral of the Lagrangian density $\mathcal{L}_E$. Here, $\tau = it$ denotes the imaginary time coordinate, compactified to the interval $[0, 1/T]$, and V is the spatial volume. The Euclidean Lagrangian density $\mathcal{L}_E$ of QCD at zero baryon chemical potential is

$$\mathcal{L}_E = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \sum_{f=1}^{N_f} \bar{\psi}_f (\gamma_\mu D_\mu + m_f) \psi_f, \quad (1.2)$$

where $D_\mu = \partial_\mu - ig A_\mu^a t^a$ is the gauge covariant derivative, with t^a representing the generators of the SU(3) color gauge group in the fundamental representation. Furthermore, $F_{\mu\nu}^a$ is the non-Abelian gluon field strength tensor, defined as

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g f^{abc} A_\mu^b A_\nu^c, \quad (1.3)$$

with g representing the strong coupling, A_μ^a the gluon fields, and f^{abc} the totally anti-symmetric structure constants of the SU(3) algebra. The fermionic fields ψ_f and $\bar{\psi}_f$ correspond to the N_f distinct quark flavors, each carrying a bare mass m_f . Because the trace in the partition function results in the compactified τ direction, it also enforces strict periodicity for bosonic gluon fields i.e. $A_\mu^a(\tau, \mathbf{x}) = A_\mu^a(\tau + 1/T, \mathbf{x})$ and the fermionic quark fields to obey strict anti-periodic boundary conditions, $\psi_f(\tau, \mathbf{x}) = -\psi_f(\tau + 1/T, \mathbf{x})$.

It is instructive to first consider the global symmetries of QCD in the limit where the N_f quark flavors are strictly massless. The classical QCD Lagrangian written in Eq. 1.2 possesses a global chiral symmetry [4] involving independent transformations of the left- and right-handed quark fields, given by

$$\mathcal{G}_{\text{classical}} = \text{SU}_L(N_f) \times \text{SU}_R(N_f) \times \text{U}_L(1) \times \text{U}_R(1). \quad (1.4)$$

This continuous symmetry group can be equivalently re-expressed in terms of vector and axial-vector transformations as $\text{SU}_V(N_f) \times \text{SU}_A(N_f) \times \text{U}_V(1) \times \text{U}_A(1)$. While the $\text{U}_V(1)$ symmetry results in the conservation of baryon number, the $\text{U}_A(1)$ axial symmetry is

explicitly broken at the quantum level by the Adler-Bell-Jackiw anomaly [5–7],

$$\partial_\mu j_5^\mu = 2iN_f q(x), \quad \text{where } q(x) = \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}^{\mu\nu,a}, \quad a = 1, \dots, N_c^2 - 1. \quad (1.5)$$

Here, $q(x)$ represents the topological charge density, and $\tilde{F}^{\mu\nu,a} = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} F_{\rho\sigma}^a$ is the dual gluon field strength tensor. Because the spacetime integral of $q(x)$ yields an integer-valued topological charge Q , this quantum anomaly inextricably links the explicit breaking of the axial symmetry to the complex, non-trivial vacuum topology of QCD. Consequently, the exact global symmetry of the full quantum theory of strong interactions in the massless limit is reduced to $SU_L(N_f) \times SU_R(N_f) \times U_V(1)$.

At $T = 0$, $\mu_B = 0$, the non-singlet subgroup of chiral symmetry in the QCD vacuum is spontaneously broken to its vector subgroup, $SU_V(N_f)$. In our physical world, the quarks are massive, and in the region of the phase diagram we are interested in, only the up, down, and strange quarks contribute to thermodynamic properties. However, since the up and down quarks are nearly degenerate in mass which are much smaller than the confining scale Λ_{QCD} , there is an explicit but minimal breaking of the chiral symmetry from the outset. Therefore, for all practical purposes related to the discussion of the QCD phase diagram, there is an almost exact $N_f = 2$ chiral symmetry in QCD. The spontaneous symmetry breaking of this $SU_L(2) \times SU_R(2)$ chiral symmetry is characterized by a non-vanishing vacuum expectation value of a scalar quark bilinear, known as the chiral condensate [8],

$$\langle \bar{\psi}\psi \rangle \equiv \langle \bar{u}u + \bar{d}d \rangle \neq 0. \quad (1.6)$$

Because it signals the spontaneous breaking of $N_f = 2$ chiral symmetry, the chiral condensate serves as the primary order parameter for the chiral phase transition.

Due to a change in the temperature and baryon densities, it is expected that the $N_f = 2$ chiral symmetry will be eventually restored at higher temperature and baryon densities to give rise to a macroscopically distinct state of matter known as the quark-gluon plasma

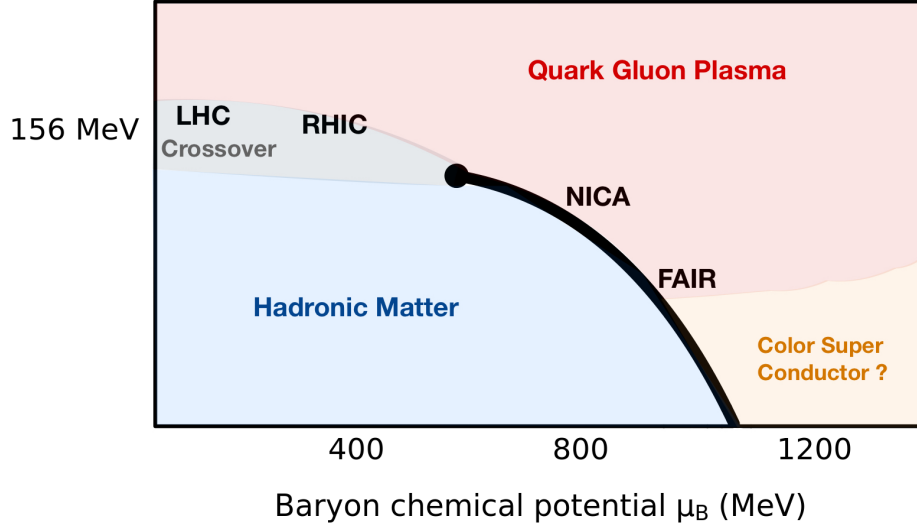


Figure 1.1: Schematic QCD phase diagram for (2+1)-flavor QCD with physical quark masses in the temperature and baryon chemical potential plane, illustrating the hadronic phase, quark-gluon plasma phase, crossover region, and the possible critical end point (shown as a black dot), followed by a first-order transition line (solid black line). Different experimental programs, such as LHC, RHIC, NICA, and FAIR, probe different regions of the QCD phase diagram.

(QGP). We know from first principles lattice QCD studies that such a transition at $\mu_B = 0$ is a smooth crossover [9–11]. This is due to the fact that a tiny breaking of the two-flavor chiral symmetry results in a smooth analytic dependence of the chiral condensate on temperature and its singular part that solely survives in the exact chiral limit is subdominant. The pseudo-critical temperature T_{pc} for the crossover can still be defined from the peak of the chiral susceptibility and the inflection point of the renormalized chiral condensate, and has been established in the continuum limit to be $T_{pc} \approx 156.5$ MeV [12–14]. Above this crossover temperature, the color degrees of freedom carried by quark and gluon are deconfined, forming a strongly interacting QGP. A schematic of possible phases for (2 + 1)-flavor QCD is shown in Fig. 1.1 as a function of temperature and baryon chemical potential. Most regions with non-vanishing μ_B are not strictly accessible via first-principles calculations due to the fermion sign problem [15], and therefore rely on extrapolation techniques from $\mu_B = 0$ or hints from effective theories [1, 16, 17] which share the same symmetries as QCD. In this thesis, we focus exclusively on the $\mu_B = 0$ region of the QCD

phase diagram at finite temperatures, near and well above the pseudo-critical temperature. Evidences [18] from lattice studies favors a second-order phase transition belonging to the 3D $O(4)$ universality class in the exact 2-flavor chiral limit ($m_f \rightarrow 0$), whereas other universality classes have not been ruled out [19, 20]. In fact the order of the chiral phase transition depends on the magnitude of $U_A(1)$ breaking [19]. In Chapter 4, we address the question of whether certain quantities carry information about the universality class of the chiral phase transition even for QCD with physical quark masses.

Another deeper question that remains unanswered is how such a strongly interacting quantum matter reaches thermal equilibrium to begin with. Indirect hints from heavy-ion collision experiments reveal a fast thermalization to a locally thermal QGP phase [21, 22]. Understanding the precise microscopic mechanism behind this rapid equilibration remains a significant theoretical challenge. While classical systems thermalize via ergodicity and chaotic dynamics, the thermalization of closed quantum systems is fundamentally understood through the Eigenstate Thermalization Hypothesis (ETH) [23]. The quantum chaos responsible for ETH leaves a critical signature in the spectral properties of the system. The Bohigas-Giannoni-Schmit (BGS) conjecture [24] states that quantum systems whose classical dynamics are chaotic are characterized by energy eigenspectra that exhibit universal level-spacing fluctuations described by one of the three Wigner-Dyson classes of random matrix theory (RMT). Conversely, the Berry-Tabor conjecture [25] states that if the classical dynamics of a system is completely integrable, then the energy eigenvalues of its quantum Hamiltonian behave like a sequence of independent random variables, following Poisson statistics. Hence it will be worth demonstrating an explicit realization of these conjectures in QCD to understand how such a strongly interacting quantum system thermalizes. This is also one of the topics addressed in this thesis, particularly in Chapter 4.

Returning to the discussion about QCD thermodynamics, the central task is to calculate the partition function defined in Eq. 1.1. The path integral near the crossover transition,

where g is non-perturbatively large, is analytically intractable. Evaluating this integral requires discretizing the continuous space-time manifold onto a four-dimensional hypercubic lattice of spacing a and performing the integration numerically using Monte Carlo techniques, a framework known as lattice QCD. However, naively discretizing the Dirac fermions on a lattice introduces severe theoretical challenges regarding the preservation of chiral symmetry. In Section 1.2, we detail the various lattice fermion formulations and the fundamental challenges associated with simulating chiral physics.

1.2 Introduction to the basics of lattice QCD

As already mentioned lattice QCD involves discretizing the QCD Lagrangian on a Euclidean box with a spacing a . In order to strictly preserve local gauge invariance on the discrete space-time, the continuum gauge fields $A_\mu(x)$ are replaced by parallel transporters defined as the links connecting adjacent lattice sites n and $n + \hat{\mu}$. These link variables are elements of the unitary $SU(3)$ group, defined as $U_\mu(n) = \exp(ia g A_\mu^a(n) t^a)$ [26]. The fermion fields $\psi(n)$ reside on the lattice sites. The gauge covariant derivative that appears in the definition of the Dirac operator is constructed by connecting fermion fields on nearest neighbor sites using gauge links $U_\mu(n)$.

The discrete version of the derivative operator is not unique. To discuss the merits of different discretization which lead to different realizations of the lattice Dirac operator, it is instructive to consider a trivial gauge background, where all links are set to the identity matrix, $U_\mu(n) = \mathbb{I}$. The naive discretization involves replacing the continuum spacetime derivative by a central derivative on the lattice. The central derivative preserves hermiticity and thus appears to be the most natural choice. Performing a Fourier transformation, the lattice Dirac operator for a single quark of mass m takes the form

$\tilde{D}(p) = ma\mathbb{I} + i \sum_{\mu=1}^4 \gamma_{\mu} \sin(p_{\mu}a)$. Its inverse, the quark propagator, is

$$\tilde{D}(p)^{-1} = \frac{ma\mathbb{I} - \sum_{\mu=1}^4 \gamma_{\mu} \sin(p_{\mu}a)}{m^2a^2 + \sum_{\mu=1}^4 \sin^2(p_{\mu}a)}. \quad (1.7)$$

In the continuum limit, the $p_{\mu}a \equiv (0, 0, 0, 0)$ should only contribute to the quark propagator. However, due to the periodicity of $\sin(p_{\mu}a)$, it goes as a $p_{\mu}a$ whenever any of the components of the momentum vector are either $ap_{\mu} = 0$ or $ap_{\mu} = \pi$. This periodic behavior thus introduces $2^4 - 1 = 15$ unphysical, redundant poles in the massless limit, located at the corners of the Brillouin zone. These unwanted artificial degrees of freedom are known as *fermion doublers*.

Any fermion discretization scheme on the lattice has to satisfy the **Nielsen–Ninomiya no-go theorem** for the Dirac operator D , which states that all the following four conditions cannot be satisfied simultaneously [27],

1. **Translation invariance:** The operator respects the discrete translational symmetries of the lattice.
2. **Locality:** The operator is strictly ultra-local or at least exponentially local. The kernel of the Dirac operator must decay at least exponentially with distance, ensuring the momentum-space operator remains a continuous and differentiable function.
3. **Absence of fermion doublers:** The massless Dirac propagator has exactly one pole at $p_{\mu}a \equiv 0$
4. **Exact chiral symmetry:** Dirac operator satisfies $\{D, \gamma_5\} = 0$.

Consequently, every lattice fermion formulation must violate at least one of these four properties. Depending on that, there are four lattice fermion formulation which are most popularly used in the lattice calculations:

Wilson Fermions eliminate these unphysical doubler states by adding a Laplacian operator that behaves like a mass term, to the naive lattice Dirac operator [26]. The matrix

elements of the Wilson Dirac operator on the spacetime lattice is defined as

$$D_W(ma)_{nm} = (ma + 4) \delta_{n,m} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{I} - \gamma_\mu) U_\mu(n) \delta_{n+\hat{\mu},m}, \quad (1.8)$$

where $\gamma_{-\mu} \equiv -\gamma_\mu$ and $U_{-\mu}(n) = U_\mu^\dagger(n - \mu)$. For a trivial gauge link $U_\mu(n) = \mathbb{I}$, in momentum space, the addition of the Laplacian modifies the propagator by a mass factor $2/a$ at every corner of the Brillouin zone. As a consequence, the doublers become infinitely heavy and completely decouple from the physical spectrum in the continuum limit [28]. However the Wilson operator by construction does not satisfy exact chiral symmetry on the lattice. When gauge interactions are turned on this leads to additive mass renormalization, requiring a precise fine-tuning of the bare quark mass m to recover the physical theory. The exact chiral symmetry is only recovered in the continuum limit.

The **staggered** fermion discretization [29,30] reduces the 16-fold degeneracy of the naive discretization down to four quark degrees of freedom, referred to as *tastes*, while successfully maintaining a remnant $U(1)$ subgroup of the original 2-flavor chiral symmetry of QCD. This is achieved by performing a diagonalization of the naive lattice Dirac operator in the spinor-flavor space which is achieved using the following transformation of the fermion fields, $\psi(n) = \gamma_1^{n_1} \gamma_2^{n_2} \gamma_3^{n_3} \gamma_4^{n_4} \psi'(n)$. Consequently, the quark action can be described using a single-component spinor field $\chi(n)$ that carries color indices. In this single-component basis, the massive staggered Dirac operator takes the form,

$$D_{n,m}^{\text{stagg}} = ma \delta_{n,m} + \frac{1}{2} \sum_{\mu=1}^4 \eta_\mu(n) \left[U_\mu(n) \delta_{n+\hat{\mu},m} - U_\mu^\dagger(n - \hat{\mu}) \delta_{n-\hat{\mu},m} \right], \quad (1.9)$$

where $\eta_\mu(n) = (-1)^{\sum_{\nu=1}^{\mu-1} n_\nu}$, with $\eta_1(n) = 1$ are the phase factors [28]. The massless staggered action preserves a continuous $U(1) \times U(1)$ chiral symmetry in the spin-taste basis such that $\{D^{\text{stagg}}, \eta_5\} = 0$ where $\eta_5(n) = (-1)^{n_1+n_2+n_3+n_4}$, with $n = (n_1, n_2, n_3, n_4)$ represents site index. Here again the exact chiral symmetry of QCD is recovered only in the continuum limit. This can be shown explicitly by reconstructing four-component

Dirac spinors in terms of these one-component fields situated at different lattice sites which leads to the emergence of a Laplacian term [28]. At finite lattice spacing, fluctuating gauge fields induce interactions between these tastes, leading to significant taste-symmetry breaking artifacts [31]. As a result, one obtains 16 flavors of pions which are split into non-degenerate multiplets due to explicit taste breaking, leaving only one exactly massless Goldstone pion in the chiral limit [32]. The full 16-fold degeneracy is only recovered in the continuum limit. To suppress these additional pions and their splitting, modern large-scale simulations employ the **Highly Improved Staggered Quark (HISQ)** action [33]. The HISQ discretization mitigates taste mixing by applying a double-smearing procedure to the gauge links and introducing a three-link Naik term to eliminate tree-level discretization errors up to $\mathcal{O}(a^2)$.

To bypass the Nielsen–Ninomiya theorem without giving up exact chiral symmetry one needs to revisit the definition of chiral symmetry on the discrete lattice. In 1982, Ginsparg and Wilson demonstrated [34] that the continuum chiral symmetry reduces to the following Ginsparg–Wilson relation by performing a coarse-graining of the continuum theory on a discrete lattice,

$$\{D, \gamma_5\} = aD\gamma_5D. \quad (1.10)$$

The chiral symmetry relation $\{D, \gamma_5\} = 0$ is clearly recovered in the $a \rightarrow 0$ limit. However on the lattice we will write the above relation in terms of lattice Dirac operator, which is dimensionless and henceforth remove any explicit mention of the lattice spacing. As a result one can define exact analogues of the chiral transformation on a finite lattice [35] and recover the anomaly relation and the Atiyah–Singer index theorem [36] even at a finite lattice spacing.

Overlap fermion [37–39] operator is an explicit solution of the Ginsparg–Wilson relation, which for massless quarks is defined as [40],

$$D_{ov} = \mathbb{I} + \gamma_5 \text{sign}[H], \quad \text{where} \quad H = \gamma_5 D_W(-M_5), \quad \text{sign}[H] = \frac{H}{\sqrt{H^2}}, \quad (1.11)$$

and D_W denotes a Wilson Dirac operator but with a negative mass parameter M_5 . Since H is a Hermitian operator, the sign function is well-defined. The parameter M_5 represents a domain wall or *defect* height and is strictly restricted to the range $0 < M_5 < 2$ for simulating one flavor of quarks [41]. In this formalism the matrix sign function neatly separates the physical quarks from the doublers, which only co-exist when $M_5 = 2, 4, 6, \dots$

While the Wilson Dirac operator $D_W(-M_5)$ in the sign function involves only nearest-neighbor terms and is a sparse matrix, evaluating the inverse square root of $D_W^\dagger D_W$ in Eq. 1.11 generates a dense matrix that has non-vanishing entries for all pairs of lattice sites n, m [42]. Consequently, $(D_{ov})_{nm} \neq 0$ for all sites, meaning the overlap operator is not ultralocal. Its kernel however decays *exponentially* fast at large distances. Because the matrix is dense, every single application of D_{ov} onto a spinor field requires evaluating the matrix sign function iteratively via high-order rational approximations. This computational burden is severely exacerbated in QCD with physical quark mass where gauge configurations with non-trivial topology frequently produce near-zero eigenvalues in the Hermitian kernel H . These near-zero modes cause the condition number to diverge, drastically increasing the required number of iterations to implement the sign function with a numerically high precision. As a result, generating large-scale dynamical gauge ensembles with overlap fermions is typically orders of magnitude more computationally demanding than utilizing standard ultra-local actions like HISQ or Wilson. Due to this extreme cost, overlap operators are primarily restricted as a valence quark operator on pre-existing gauge ensembles or are used in dynamical simulations in a fixed topological sector [43]. This computational bottleneck naturally motivates the use of domain wall fermions, which respect chiral symmetry to a very good extent on a finite lattice.

Domain wall fermion (DWF) formulation describes a massless quark in five dimensional Euclidean spacetime in the presence of a domain wall (or a defect) along the fictitious fifth dimension. The four dimensional fermions remain confined on the defect and interact with four-dimensional gauge fields $A_\mu(x)$. The five-dimensional Dirac equation can be

written as [44],

$$\left[\not{D} + \gamma_5 \partial_s + m(s) \right] \Psi_{\pm}(x, s) = 0, \quad (1.12)$$

where $\not{D}$ is the 4D covariant derivative, and $m(s)$ is a defect introduced along the fifth dimension. We choose a particular definition of the defect where $m(s) = M_5 \epsilon(s)$ with domain-wall height $M_5 > 0$. Since there are no interacting term along the fifth dimension, the five-dimensional spinor can be separated into $\Psi_{\pm}(x, s) = \psi(x) \phi_{\pm}(s)$ where $\psi(x)$ is the usual 4D wavefunction for a massless quark such that $\not{D}\psi(x) = 0$. The $\phi_{\pm}(s)$ are the eigenstates of γ_5 such that $\gamma_5 \phi_{\pm} = \pm \phi_{\pm}$. Substituting them in Eq. 1.12 we obtain the explicit solutions of $\phi_{\pm}$ which are

$$\phi^+(s) = N \exp(-M_5 |s|) \quad \text{and} \quad \phi^-(s) \propto \exp(M_5 |s|). \quad (1.13)$$

There is only one normalizable solution $\phi^+(s)$ which is exponentially localized at the defect site $s = 0$ and Ψ_+ represents a right-handed quark whose 4D wavefunction is $\psi(x)$. Conversely, the left-handed mode $\phi^-(s)$ is non-normalizable. The overlap between the left and right chiral states at tree-level is quantified in terms of a residual mass $m_{\text{res}} \sim e^{-2M_5 L_5}$ which vanishes in the limit of infinite fifth dimension $L_5 \rightarrow \infty$.

On a finite lattice the continuous fifth dimension is discretized into N_5 sites with a spacing a_5 such that the total extent $L_5 = a_5 N_5$. The domain wall operator is constructed out of the four-dimensional Wilson Dirac operator D_W with a negative domain-wall height M_5 , and a central derivative term D_5 , along the fifth dimension [45],

$$D_{s,x,s',y}^{\text{DWF}} = \delta_{s,s'} D_W(-M_5)_{xy} + \frac{a}{a_5} \delta_{x,y} (D_5)_{s,s'}. \quad (1.14)$$

Crucially, the gauge links within D_W are purely four-dimensional i.e. there are no gauge interactions along the fictitious s -direction. The operator D_5 can be specifically written in terms of left and right chiral projection operators $P_{L,R} = \frac{1}{2}(\mathbb{I} \mp \gamma_5)$ and the bare quark mass

as,

$$\begin{aligned} (D_5)_{s,s'} &= \delta_{s,s'} - (1 - \delta_{s,L_5-1})P_L\delta_{s+1,s'} - (1 - \delta_{s,0})P_R\delta_{s-1,s'} \\ &+ ma(\delta_{s,L_5-1}P_L\delta_{0,s'} + \delta_{s,0}P_R\delta_{L_5-1,s'}) . \end{aligned} \quad (1.15)$$

The physical four-dimensional quark fields $\psi(x)$ and $\bar{\psi}(x)$ can be constructed from these five dimensional wavefunctions using the following equations

$$\begin{aligned} \psi(x) &= P_L\Psi(x,0) + P_R\Psi(x,L_5-1) , \\ \bar{\psi}(x) &= \bar{\Psi}(x,L_5-1)P_L + \bar{\Psi}(x,0)P_R . \end{aligned} \quad (1.16)$$

The five-dimensional DWF action not only contains these physical fields but also unphysical contributions due to heavier bulk modes. One can isolate the contributions of these heavy so-called Pauli-Villars modes [46], by choosing anti-periodic boundary conditions along the fifth dimension implemented by setting the quark mass $ma = 1$. Integrating over the fermionic and Pauli-Villars fields yields a partition function given by a ratio of determinants, which is equivalent to a truncated overlap operator $D_{ov,L_5}(m)$ [46, 47] defined at a finite L_5 ,

$$\frac{\det[D_{\text{DWF}}(ma)]}{\det[D_{\text{DWF}}(ma=1)]} = \det[D_{ov,L_5}(ma)] . \quad (1.17)$$

If the extent of the fifth dimension L_5 is infinitely large $L_5 \rightarrow \infty$, the sign function approximation becomes exact and the overlap operator $\det[D_{ov}(m)]$ is recovered. For a finite fifth dimensional extent however the left and the right handed quark zero modes have a significant overlap which for smooth gauge backgrounds should vanish only for $L_5 \rightarrow \infty$ limit. The distinct advantage of the domain wall formalism is that the chiral and continuum limits are now clearly disentangled. However one needs to perform simulations with a finite and reasonably large L_5 increasing its computational cost compared to Wilson or staggered fermions.

In order to minimize the mixing between the left and right handed modes even on a finite fifth dimensional extent, the **Möbius Domain Wall Fermion (MDWF)** action was developed [48,49]. Instead of the conventional Hermitian Dirac operator $\mathcal{H} = \gamma_5 D_W(-M_5)(2 + D_W(-M_5))^{-1}$ that enters into the definition of the transfer matrices that communicate between the neighboring four dimensional slices along the fifth dimension, the MDWF relies on,

$$\mathcal{H}^{\text{Möbius}} = \gamma_5 \frac{(b_5 + c_5) D_W(-M_5)}{2 + (b_5 - c_5) D_W(-M_5)}, \quad (1.18)$$

where b_5, c_5 are the real Möbius parameters which follow the relation $b_5 - c_5 = 1$ and $b_5 + c_5 > 1$. The Möbius parameters effectively stretch the fifth dimensional extent from $L_5 \rightarrow L_5(b_5 + c_5)$ [50]. This allows MDWF to have a smaller chiral symmetry violation quantified in terms of m_{res} compared to traditional DWF with the same L_5 .

To complete the definition of the QCD action one has to discretize the gluon action on the lattice in a gauge invariant manner. The most fundamental discretization of $\text{SU}(N_c)$ gauge fields results in the standard Wilson gauge action [26], which is constructed out of elementary square plaquettes defined as $P_{\mu\nu}(n) = \mathcal{P} [U_\mu(n) U_\nu(n + \hat{\mu}) U_\mu^\dagger(n + \hat{\nu}) U_\nu^\dagger(n)]$, where $\mathcal{P}$ denotes path ordering, as

$$S_W^G = \frac{2N_c}{g^2} \sum_n \sum_{\mu < \nu} \left(1 - \frac{1}{N_c} \text{Re tr}[P_{\mu\nu}(n)] \right). \quad (1.19)$$

While the Wilson action is the simplest example of a discretized gauge action, it has finite $\mathcal{O}(a^2)$ cut-off errors which are comparatively large for modest lattice spacings. This has important consequences for studying topological fluctuations of the QCD vacuum. The anomalous $U_A(1)$ symmetry is related to the change in the topological charge via the index theorem [51], which is a strictly integer-valued invariant in the continuum. However on a lattice, the fundamental quantities are gauge links which can be smoothly connected to the identity element of the group, thus making it difficult to identify the topologically non-trivial gauge configurations. One can instead identify non-trivial topology on the lattice from the zero modes of the lattice Dirac operators which satisfy the index theorem

even on a finite lattice spacing. In order to satisfy the index theorem the gauge fields should be sufficiently smooth i.e., the dominant lattice cut-off effects should be exactly canceled through improvement of the gauge action. One such example is the **Iwasaki gauge action** [52] which is defined as,

$$S_{\text{Iwasaki}}^G = \frac{2N_c}{3g^2} \sum_n \left(c_0 \sum_{\mu < \nu} \text{Re tr} [\mathbb{I} - P_{\mu\nu}(n)] + c_1 \sum_{\mu \neq \nu} \text{Re tr} [\mathbb{I} - R_{\mu\nu}(n)] \right). \quad (1.20)$$

The matrix $\mathbb{I}$ denotes the 3×3 identity matrix in color space. The coefficients c_0 and c_1 are the relative weights of the plaquette and 1×2 rectangular loops $R_{\mu\nu}$ respectively, chosen such that the tree-level $\mathcal{O}(a^2)$ discretization is exactly canceled. This leads to the constraint $c_0 + 8c_1 = 1$. For the practical simulations with MDWF discussed in Chapter 3 and Chapter 4, the rectangular weight is fixed to $c_1 = -0.331$, thus $c_0 = 3.648$. Finally to construct the partition function one needs to integrate over the links, which is done using the gauge invariant Haar measure [53].

Having discussed the necessary lattice techniques that go into the definition of the QCD action, we will now study the eigenspectrum of the four dimensional Dirac operator which appears in the action. We will use either the HISQ discretization, which preserves a remnant subgroup of the continuum (almost) exact 2-flavor chiral symmetry, or the overlap discretization which has an exact chiral symmetry on the lattice to probe the thermodynamic and transport properties of QCD. In the next section, we motivate why a precision lattice study of the properties of the lattice Dirac spectrum is important for understanding the effective restoration of different subgroups of chiral symmetry and localization phenomena.

1.3 The importance of understanding the QCD Dirac eigenspectrum

The eigenvalue spectrum of the Dirac operator provides important insights regarding the symmetries of QCD and their breaking. An eigenstate of the Dirac operator describes a one-particle massless *quark state* in the presence of a gauge background. Gauge fields provide both interactions and the disorder whose strength varies as a function of temperature. Properties of the eigenvalue spectrum of the QCD Dirac operator, in the presence of gauge ensembles, have been studied extensively on the lattice both at zero as well as finite temperatures.

In the spontaneously broken phase of chiral symmetry, the spectral density $\rho(\lambda \rightarrow 0)$ of near-zero eigenvalues of the massless Dirac operator yields a precise estimate of the chiral condensate through the Banks Casher relation [54]. The chiral condensate serves as the exact order parameter for the breaking of the non-singlet subgroup of chiral symmetry in QCD in the limit of massless quarks. At temperatures $T < T_{pc}$ the level statistics of the most infrared eigenvalues of the Dirac operator can be explained within the universality class of RMT consisting of chiral Gaussian unitary ensemble (GUE) [55–58] whereas for the so-called bulk eigenvalues, the universal features can be explained within Wigner’s classification with a RMT ensemble of conventional Gaussian unitary type.

At higher temperatures, the non-singlet subgroup of the almost exact two-flavor chiral symmetry is *effectively* restored at T_{pc} i.e., the disconnected part of the chiral susceptibility matches with the topological susceptibility divided by m^2 , where m is the mass of degenerate light quark flavors [59,60]. This also leads to perceptible changes in the eigenvalue spectrum of the Dirac operator, the intercept $\rho(0)$ vanishes, leading to the formation of a small peak-like feature in the deep infrared part of the eigenvalue spectrum. This peak-like feature has been observed in studies using a mixed-action set-up [61–63] which

was debated for a while [64–67]. However, the existence of the peak-like feature was shown with dynamical domain wall fermions [68] on a finite lattice, now also observed to survive in the continuum limit in 2+1 flavor QCD with HISQ discretization [69]. In Chapter 2 we discuss how this peak-like feature in the deep infrared region of the Dirac eigenspectrum leads to the breaking of the $U_A(1)$ just above the crossover temperature, which is quite unlike the remnant breaking that persists at asymptotically high temperatures.

The larger (bulk) eigenvalues whose density grows linearly with λ are disordered i.e., their level spacing ratios are consistent with the predictions from RMT belonging to the GUE. The peak-like feature and bulk spectrum overlap strongly, resulting in the most infrared eigenmodes to be delocalized [70–72] but not ergodic, since their inverse participation ratio does not scale inversely with volume. Their level spacing fluctuations are intermediate between the Poissonian and GUE values [73, 74]. These infrared eigenmodes are characteristic of a strongly-coupled regime [70, 75, 76] and exhibit fractal-like features [73]. The median of the distribution of fractal dimensions for these *intermediate* eigenvalues is similar to that for the order parameter near the critical point of an $O(4)$ spin model [73]. Details about these findings are discussed in Chapter 4. In contrast, bulk eigenstates are ergodic since their inverse participation ratios scale as $\sim L^{-2.8}$ [73] and are thus delocalized over the entire volume.

The $U_A(1)$ subgroup is *effectively* restored at a temperature, $T_{U(1)}$, when physical observables which are sensitive to it, e.g., the topological susceptibility has a temperature dependence which is consistent with the expectation from a dilute gas of instantons [60]. This can be motivated by the fact that once an onset to the dilute instanton gas regime occurs, there are no further changes in the topological properties even when temperatures are increased to asymptotically large values. The $T_{U(1)}$ is close to $\gtrsim 1.5 T_{pc}$ inferred from the temperature dependence of the topological susceptibility in QCD [59], from the features in the Dirac eigenvalue spectrum [61, 72], from the degeneracy of temporal meson

correlators [77] and from a renormalized ratio of the meson susceptibilities [78, 79]. At comparatively smaller lattice of spatial size $\lesssim 2.4$ fm and in the continuum limit, however an effective restoration of $U_A(1)$ is observed in the isotriplet meson channel close to T_{pc} [80] even though such a restoration has not been observed in the isosinglet channel. A weaker bound $T_{U(1)} \gtrsim 1.2 T_{pc}$ was obtained from the fact that values of $\chi_\pi - \chi_\delta$ arising due to the mixing between near-zero eigenvalues with the bulk vanishes at this temperature [69], details of the calculations can be found in Section 2.4. Temperature dependence of the topological susceptibility measured from the zero modes of the overlap Dirac operator is discussed in detail in Chapter 3.

The scenario at even higher temperatures $T > T_{U(1)}$ is not yet well understood. Whereas a peak-like feature of near-zero eigenmodes similar to $m^2\delta(\lambda)$ should survive, expected from a dilute gas model for instantons [61, 72, 81, 82], it is heavily suppressed as a function of temperature. Thus its contribution to topological susceptibility decreases as $\sim T^{-8}$ [59, 83, 84]. Eventually, these infrared eigenmodes should be gapped out from the bulk part of the eigenvalue spectrum. Recent studies indicate that at sufficiently high temperatures, the most infrared part of this bulk spectrum contains localized eigenvalues which can be distinguished from the other delocalized bulk eigenmodes, which follow GUE level statistics, through a mobility edge [63, 85, 86]. This phenomenon is analogous to a localization transition [63, 86–91] observed in the Anderson model [92], where random matrix ensembles interpolate between Poisson and Wigner-Dyson statistics close to the mobility edge. In this regime critical eigenstates exhibit sparse, fractal-like structures. They are strongly correlated for very closely spaced eigenvalues but weakly correlated for large separations. Examining whether infrared eigenmodes of the QCD Dirac operator are fully ergodic with level spacing fluctuations consistent with RMT or there persists localized eigenstates provides insights into whether strongly interacting QGP shows signatures of many-body localization, which should manifest as an Anderson-like transition [93]. Nonetheless, a naive Anderson-like scaling of its temperature dependence demonstrates that the mobility edge might vanish at the pseudo-critical temperature [63, 87, 94], but

it might also disappear only at the critical temperature which is achieved in the chiral limit [86]. The robustness of these observations needs to be tested through carefully performed infinite volume and continuum extrapolations.

To summarize, whereas there is a wealth of results on spectral signatures related to *effective* restoration of the different subgroups of chiral symmetry, and on the localization properties manifest as an Anderson-like transition, separately, the interplay between these two physically distinct phenomena is not so clear. We want to emphasize here that these two phenomena have distinct physical origins and thus their consequences will also be different. The Anderson transition is a quantum phase transition which, strictly speaking, is a zero-temperature one-particle phenomenon. A possible way to understand such a (de-)localization transition at finite temperatures is to attribute the change in the strength of the disorder in terms of gauge fluctuations arising due to a change in temperature however, a clear connection between the two is not very apparent.

In QCD, varying the temperature also results in the sequential (effective) restoration of different subgroups of chiral symmetry. Evidence suggests that the restoration of the $SU_A(2)$ occurs through a second-order phase transition in the chiral limit [18], remnant effects of which will remain manifest in the Dirac eigenvalue spectrum even for physical light quarks [73]. The effective restoration of $U_A(1)$ will result in characteristic changes in the localization properties of the Dirac eigenvectors; on the other hand, an Anderson-like transition also results in structural changes in the eigenvectors of the Dirac operator. It is thus imperative to disentangle these two phenomena and unambiguously identify the mechanism that drives them. However, the temperature regimes where these occur overlap with each other, which makes it challenging to unambiguously distinguish between these two effects. The main theme of my thesis is to calculate the Dirac eigenspectrum from first principles using quarks with exact or nearly exact chiral symmetry on the lattice in order to disentangle the effects due to restoration of different subgroups of chiral symmetry from the underlying localization phenomenon.

Chapter 2

Eigenspectrum of the HISQ Dirac operator and the $U_A(1)$ anomaly

2.1 Introduction

Though the chiral crossover transition which is related to the effective restoration of the non-singlet subgroups of the almost exact 2-flavor chiral symmetry is well studied on the lattice [12], tracking the amount of anomalous $U_A(1)$ breaking on the lattice is a more subtle and difficult problem. The eigenvalue spectrum of the quark Dirac operator serves as a primary tool for understanding the effective restoration of the non-singlet subgroup of chiral symmetry, where the density of near-zero eigenvalues is directly related to the chiral condensate [54].

Lattice studies exploring the $U_A(1)$ restoration historically started with the quenched approximation of QCD and then used dynamical QCD configurations. Since $U_A(1)$ is an anomalous subgroup of the chiral symmetry in QCD related to the topology of the gauge fields via the index theorem, it is important to use fermion discretizations on the lattice which has exact chiral symmetry and an exact index. Staggered fermion discretization, which is most popularly used for the study of QCD thermodynamics, breaks the con-

tinuum chiral symmetry. The spin and flavor degrees of freedom intermingle at finite lattice spacings and thus the continuum chiral symmetries are only recovered and realized in the continuum limit. This chapter presents a systematic study of the eigenvalue spectrum of the QCD Dirac operator realized using the Highly Improved Staggered Quark (HISQ) discretization on the lattice. Performing a careful continuum extrapolation, we will discuss the fate of the $U_A(1)$ symmetry in $2 + 1$ flavor QCD across the chiral crossover transition and interpret our results in terms of the infrared part of the Dirac spectrum.

2.2 Details of the numerical lattice calculations

The numerical analysis presented in this chapter uses $2 + 1$ flavor QCD gauge configurations with physical quark masses, generated by the HotQCD collaboration [12, 95] using the Highly Improved Staggered Quark (HISQ) action for quarks and a tree-level Symanzik improved gauge action. The quark masses are tuned such that the Goldstone pion mass is 140 MeV and a kaon mass of 435 MeV. In order to systematically investigate the eigenvalue spectrum across the chiral crossover transition, we analyze five different temperatures, one below the pseudo-critical temperature T_{pc} and four above it. We then perform a continuum extrapolation of different physical observables at each temperature $T = \frac{1}{N_\tau a}$ using three temporal lattice extents $N_\tau = 8, 12$, and 16. The spatial size of the lattice is chosen such that $N_s = 4N_\tau$ ensuring that the spatial length $\gtrsim 4$ fm is maintained for all temperatures, ensuring that the physical system remains sufficiently close to the thermodynamic limit. At each temperature and lattice spacing we perform statistical averaging with 240-3390 independent gauge configurations which are separated by 50 RHMC steps. The relevant details are explicitly mentioned in Table 4.1. Using the implicitly restarted Lanczos algorithm, we extracted the lowest 200, 100, and 60 eigenvalues of the massless HISQ Dirac matrix for the $N_\tau = 8, 12$, and 16 lattices, respectively. The eigenvalue density was calculated in bins of eigenvalues of uniform size $\lambda a = 0.001$ for all temperatures and lattice spacings, and jackknife resampling was performed in order to

eliminate autocorrelation bias within the binned data.

T (MeV)	β	N_s	N_τ	N_{confs}
145	6.285	48	12	1530
145	7.010	64	16	2860
162	6.423	32	8	250
162	6.825	48	12	1960
162	7.130	64	16	3390
166	6.445	32	8	400
166	6.850	48	12	2100
166	7.156	64	16	2190
171	6.474	32	8	280
171	6.880	48	12	1980
171	7.188	64	16	1040
176	6.500	32	8	240
176	6.910	48	12	330

Table 2.1: Number of configurations for different temperatures (or equivalently the bare inverse coupling $\beta = 6/g^2$) and the corresponding lattice sizes used in this work.

2.3 General features of the QCD Dirac eigenvalue spectrum in the continuum limit

Characterizing the eigenvalue density

At zero-temperature, the Dirac eigenvalue density $\rho(\lambda)$ in QCD with N_f massless quarks can be calculated within chiral perturbation theory [54], which at linear order in λ is,

$$\rho(\lambda) = \frac{\langle 0 | \bar{\psi} \psi | 0 \rangle}{\pi} + |\lambda| \langle 0 | \bar{\psi} \psi | 0 \rangle^2 \frac{N_f^2 - 4}{32\pi^2 N_f F_\pi^4} + \dots \quad (2.1)$$

The intercept of this bulk density is related to the chiral condensate $\langle 0 | \bar{\psi} \psi | 0 \rangle$, while the ratio of the slope to the intercept is also proportional to it. At finite temperatures constraints on the $\rho(\lambda)$ exist in the chiral symmetry restored phase of QCD [96] whereas below T_{pc} , the presence of a non-zero intercept in $\rho(\lambda)$ as a function of λ is expected.

To characterize the properties of the Dirac eigenspectrum obtained using the HISQ discretization, it is essential to perform a careful continuum extrapolation. Focusing on the lowest temperature $T = 145$ MeV, the eigenvalue density is shown in the top-left panel of Fig. 2.1 for different lattice spacings. Utilizing the two available lattice spacings at this temperature to perform a continuum estimate, the chiral condensate extracted from the intercept is $\langle 0|\bar{\psi}\psi|0\rangle/T^3 = 18.4$. Concurrently performing a linear fit to the continuum estimates, the squared condensate can be extracted from the slope (setting $N_f = 3$ and $F_\pi = 94.14$ MeV), resulting in $\langle 0|\bar{\psi}\psi|0\rangle/T^3 = 17.3$, which is consistent within errors with its value extracted from the intercept. These values of chiral condensate agrees with the continuum extrapolated value of 18.8 calculated independently from the partition function by performing the trace of the inverse Dirac operator using stochastic noise vector on a larger set of HotQCD ensembles [97].

In the chiral symmetry restored phase of QCD described by $T > T_{pc}$, the bulk eigenvalue density can be parameterized as a polynomial in λ [96]:

$$\frac{\rho(\lambda)}{T^3} = \frac{\rho_0}{T^3} + \frac{\lambda}{T} \cdot \frac{c_1(T, m)}{T^2} + \frac{\lambda^2}{T^2} \cdot \frac{c_2(T, m)}{T} + \frac{\lambda^3}{T^3} c_3(T, m) . \quad (2.2)$$

In this expression, c_1 and c_2 describe the coefficients of the terms which are linear and quadratic in λ respectively, whereas the λ^3 dependence is perturbative in origin. ρ_0 denotes the intercept representing the chiral condensate. These coefficients generally depend on both the temperature T and the light quark mass m .

The temperature dependence of the normalized density $\rho(\lambda)/T^3$ above T_{pc} is illustrated in Fig. 2.1. Data from the finest lattice ($N_\tau = 16$) distinctly reveal two separated spectral features: an accumulation of near-zero eigenvalues forming a peak, and a linearly rising tail corresponding to the bulk eigenmodes. While these two features overlap significantly just below T_{pc} , making them indistinguishable, at higher temperatures the bulk eigenvalues disentangle from the deep-infrared part of the spectrum, allowing for near-zero eigenmodes to be distinctly visible. At $T > T_{pc}$ the near-zero peak is smeared due to con-

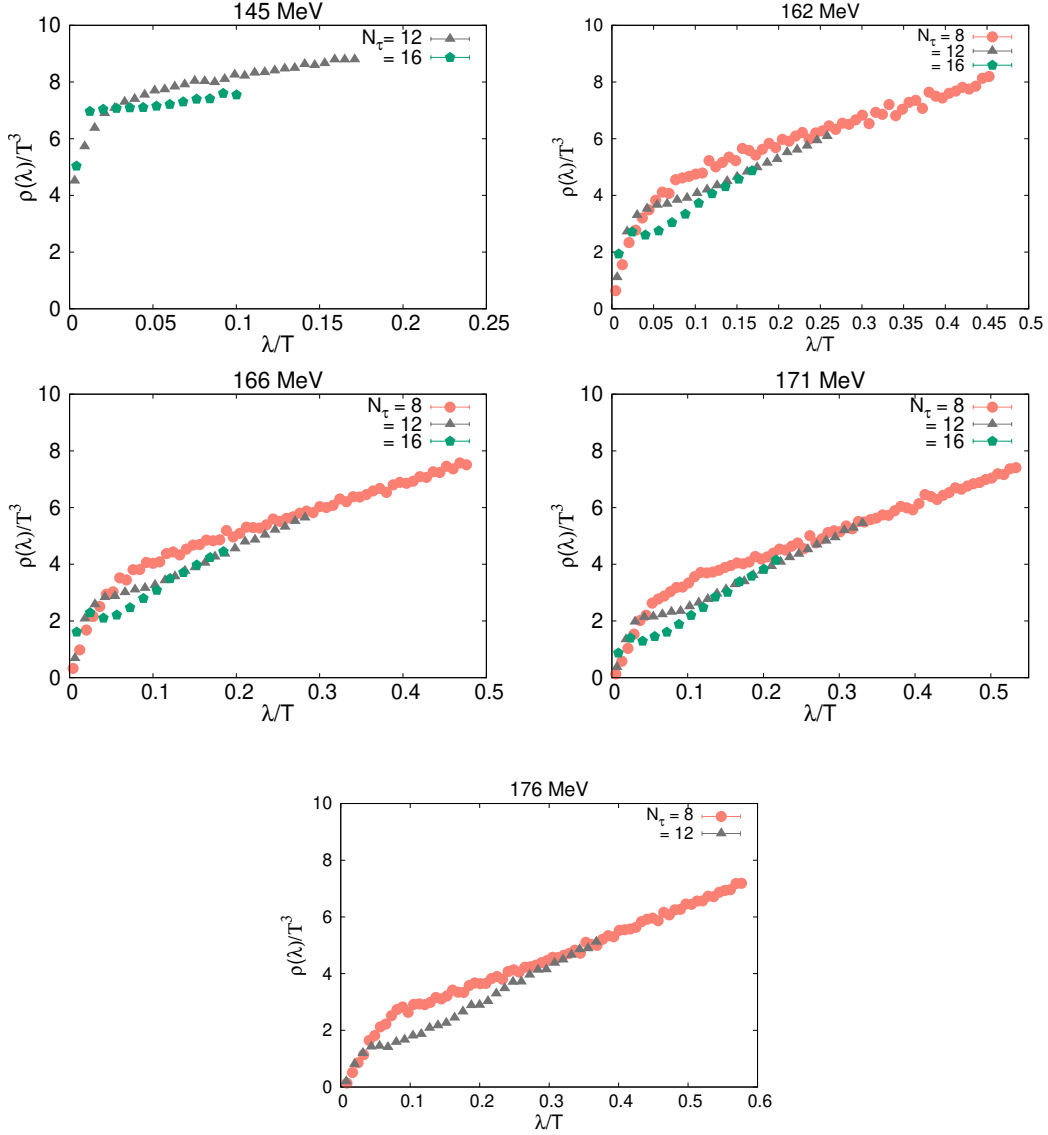


Figure 2.1: Eigenvalue spectrum for HISQ Dirac operator for three different lattice spacings corresponding to $N_\tau = 8, 12, 16$ at $T = 162, 166, 171$ MeV, for two different lattice spacings, $N_\tau = 12, 16$ at $T = 145$ MeV and $N_\tau = 8, 12$ at $T = 176$ MeV.

tamination from the bulk eigenmodes on coarser lattices but becomes distinctly visible as one approaches the continuum limit, signifying that it is a genuine physical feature rather than a discretization artifact.

To understand the origin of low-lying IR Dirac eigenmodes for temperature $T < T_{pc}$, it is instructive to draw comparisons with chiral random matrix theory (cRMT). At zero temperature, the density of scaled eigenvalues ($c\lambda$) for a two-flavor Dirac operator in the zero topological charge sector follows [98] is given as,

$$\rho(c\lambda) = \frac{c\lambda}{2} \left[J_2^2(c\lambda) - J_3(c\lambda)J_1(c\lambda) \right]. \quad (2.3)$$

By defining a dimensionful scaling parameter $c = V\langle 0|\bar{\psi}\psi|0\rangle/T$ at each T in terms of the spatial volume V and finite-temperature condensate values taken from Ref. [97], we can directly map our lattice results onto this cRMT prediction. However for a meaningful comparison the eigenvalues are rescaled further so that the first moment of the probability distribution of the lowest eigenvalue matches that of Eq. 2.4. The resulting near-zero mode distributions for $T = 145, 162, 166$, and 171 MeV are compared in Fig. 2.2. At $T = 145$ MeV, the lattice data is in good agreement with the cRMT prediction and successfully describe the initial oscillatory behavior of the small eigenvalue density with respect to $c\lambda$. Interestingly, a similar comparison with Eq. 2.3 was previously performed with Dirac eigendensity calculated in a background simulated from the instanton liquid model (ILM) at $T = 0$ [57]. As thermal effects are introduced, the ILM studies show that these density oscillations are smeared over a characteristic length scale of roughly $1/T$ [99], a phenomenon that qualitatively matches the broadened profiles we observe for our lattice data at temperatures above T_{pc} .

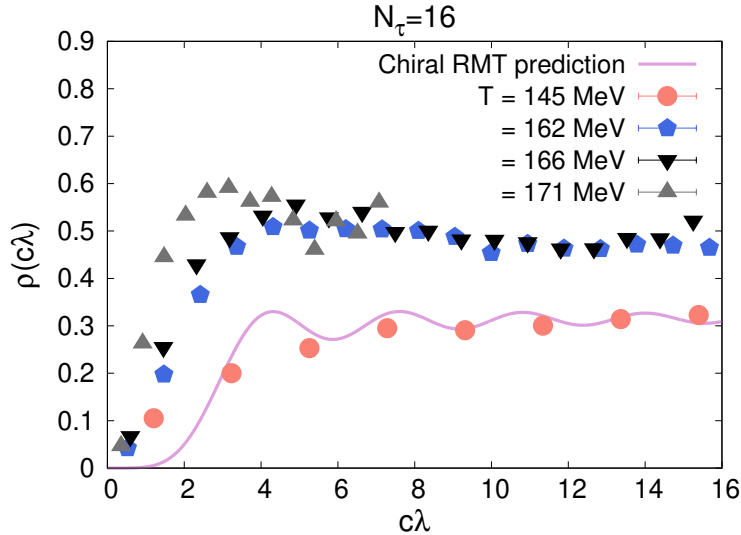


Figure 2.2: Near-zero (scaled) eigenvalue density for HISQ Dirac operator at $T = 145, 162, 166, 171$ MeV for the finest lattice spacing corresponding to $N_\tau = 16$ and its comparison with cRMT prediction available at $T = 0$.

Focusing on the bulk eigenmodes within the symmetry-restored phase, chiral Ward identities and analyticity in m^2 impose specific constraints on the Dirac eigendensity and for the effective restoration of the $U_A(1)$ anomaly [96]. Specifically, degeneracy between up to six-point scalar and pseudo-scalar correlation functions requires that $c_{1,2} = \mathcal{O}(m^2) + \dots$ and $c_3 = c_{30} + \mathcal{O}(m^2) + \dots$. While the presence of mass-independent coefficient c_{30} in the perturbative λ^3 term does not induce $U_A(1)$ breaking [96], we must investigate non-perturbatively whether $c_{1,2}$ indeed has no mass-independent constants. In order to do so, we fit the bulk spectrum defined by eigenvalues $\lambda > \lambda_0$ with a truncated version of Eq. 2.2, retaining only the intercept and the linear term. Neglecting higher powers of λ is justified since the analysis is restricted to the deep infrared regime containing roughly $\mathcal{O}(100)$ eigenvalues out of millions available on these lattice volumes. The extracted fit parameters, summarized in Table 2.2, are then continuum extrapolated using $\sim 1/N_\tau^2$ ansatz.

T [MeV]	N_τ	λ_0/T	$\frac{c_1}{T^2}$	ρ_0/T^3
145	12	0.1	9.0(5)	7.30(7)
145	16	0.05	9(1)	6.67(9)
162	8	0.2	8.8(3)	4.1(1)
162	12	0.15	13.2(2)	2.69(5)
162	16	0.1	17.5(5)	1.93(7)
166	8	0.2	8.9(1)	3.31(5)
166	12	0.15	13.3(3)	1.92(6)
166	16	0.1	16.6(8)	1.4(1)
171	8	0.2	9.3(1)	2.38(5)
171	12	0.15	12.9(1)	1.19(3)
171	16	0.1	17.0(5)	0.45(8)
176	8	0.2	9.5(1)	1.67(4)
176	12	0.15	13.0(2)	0.36(6)

Table 2.2: Lattice sizes ($N_s^3 \times N_\tau$), temperatures (T), the estimated values of c_1/T^2 and ρ_0/T^3 after the fit to the bulk eigenmodes defined beyond the lower cutoff at λ_0/T .

The continuum extrapolated values of $c_1(m, T)/T^2$ are shown as black points in Fig. 2.3.

We then fit the data to $c_1(m, T)/T^2 = \text{constant}$ and to a functional form of the type

$c_1(m, T)/T^2 = c_{12} \frac{m^2}{T^2} + c_{14} \frac{m^4}{T^4}$. The former fit with $\chi^2/\text{d.o.f} = 0.6$ is favored over the fit function that has a leading-order m^2 dependence ($\chi^2/\text{d.o.f} = 0.1$). One obtains $c_1(m, T)/T^2 =$

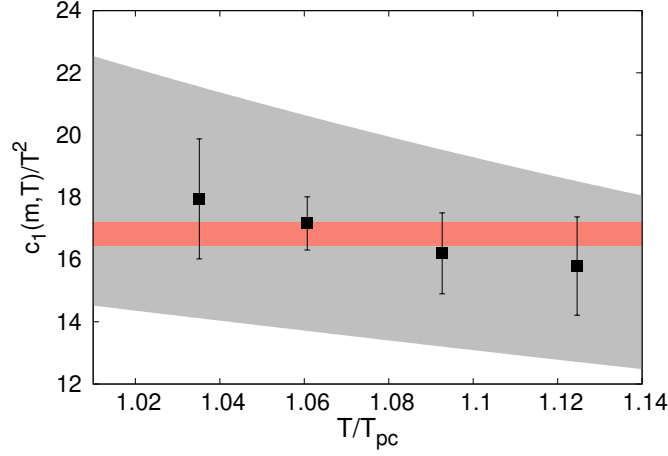


Figure 2.3: Continuum estimates for $c_1(m, T)/T^2$ for $T > T_{pc}$ obtained after fitting the points with an m -independent constant (orange band) and a sum of quadratic (m^2/T^2) and quartic (m^4/T^4) dependent fit function (gray band).

16.8(4) as a result of the fit. This indicates that the anomalous $U_A(1)$ breaking persists in the chiral symmetry-restored phase even in the strict chiral limit. As will be detailed in the subsequent section, the dominant source of $U_A(1)$ breaking comes however from the near-zero eigenvalues. Note that for temperatures $T \lesssim 1.12 T_{pc}$, the linear slope of the Dirac eigenvalue density is an indication of the non-perturbative nature of the QCD Dirac spectrum, in contrast to the standard perturbative λ^3 behavior.

Distribution of the lowest eigenvalue at finite temperature

The probability distribution of the lowest eigenvalue of the QCD Dirac operator, $\lambda_{\min}$, encodes information regarding the chiral symmetry breaking pattern in QCD. To verify that it is indeed true for the HISQ Dirac operator, we compare the continuum extrapolated distribution of the lowest eigenvalue at temperatures across the chiral crossover with the analytical prediction from cRMT. For a $N_f = 2$ chiral RMT ensemble at zero temperature, the probability distribution of the scaled lowest eigenvalue is given by [98],

$$P(x) = \frac{x}{2} e^{-\frac{x^2}{4}} \left[J_2^2(x) - J_3(x)J_1(x) \right], \quad \text{where} \quad x = c\lambda_{\min}. \quad (2.4)$$

To facilitate a direct comparison with cRMT, we examine the lowest eigenvalues across multiple lattice spacings, $N_\tau = 12, 16$ for $T = 145$ MeV, and $N_\tau = 8, 12, 16$ for $T = 171$ MeV. The minimum eigenvalues are scaled by the dimensionless variable c defined earlier in order to construct the probability distribution of $c\lambda_{\min}$ for each N_τ . We then perform a smooth interpolation of the distribution using an error-weighted cubic spline, subsequently extrapolating to the continuum limit at each value of $c\lambda_{\min}$ using the standard $c + d/N_\tau^2$ ansatz. For the $T = 145$ MeV data, where only two lattice spacings are available, we assign 15% systematic uncertainty to the extrapolation to account for the limited data set. For a proper comparison of lattice data with the cRMT prediction in Eq. 2.4, we have to ensure that both distributions must have the same first moment. We first analytically determine the first moment of the cRMT distribution to be 4.344. Consequently, we scale the $c\lambda_{\min}$ calculated on the lattice such that the first moment of its probability distribution at different temperatures exactly matches to 4.344, while ensuring the total area under the curve remains unity.

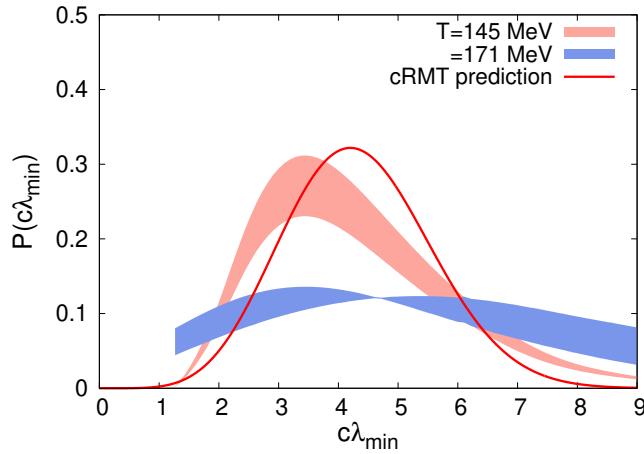


Figure 2.4: The continuum extrapolated probability distribution of the scaled lowest eigenvalue for $T = 145$ and 171 MeV, shown as orange and blue bands respectively. These are compared with the cRMT prediction for $N_f = 2$, which belongs to the GUE class.

The resulting continuum extrapolated distributions are presented in Fig. 2.4. Just below the pseudo-critical temperature at $T = 145$ MeV, the continuum distribution shown as an orange band closely agrees with the prediction from the $N_f = 2$ chiral Gaussian Unitary

Ensemble (chGUE). In contrast, at $T = 171$ MeV, the distribution shown as a blue band deviates from the zero temperature chGUE prediction. This demonstrates that the lowest eigenvalue of the QCD Dirac operator, which forms the near-zero peak at $T > T_{pc}$, is very distinct from those described by the conventional chiral GUE at zero temperature.

Universal level spacing fluctuations of the bulk eigenmodes

To understand the properties of bulk eigenmodes, we study the universal fluctuations in their level spacing distribution through the usual procedure of *unfolding*. Let λ be the eigenvalues sorted in ascending order for a given gauge configuration. The average density of these eigenvalues is denoted as $\bar{\rho}(\lambda)$. We unfold the sequence using the average staircase function,

$$\bar{\eta}(\lambda) = \int_{\lambda_0}^{\lambda} d\lambda' \bar{\rho}(\lambda'), \quad (2.5)$$

which counts the average number of eigenvalues between λ and λ_0 , which defines the beginning of the bulk spectrum. The unfolded eigenvalues are defined as $\lambda_i^{uf} = \bar{\eta}(\lambda_i)$, where i is the index of the original eigenvalue sequence. After unfolding, the average spacing between the eigenvalues is exactly unity.

Next, we calculate the separation between consecutive unfolded eigenvalues denoted by $s_i = \lambda_{i+1}^{uf} - \lambda_i^{uf}$. By grouping these s_i into small bins, we construct the nearest neighbor spacing distribution which shows the fluctuations of the level spacings about its average value. The unfolded level spacing distribution for different lattice spacings corresponding to $N_\tau = 8$ and 12 are compiled in Fig. 2.5 at each temperature $T = 162, 166, 171, 176$ MeV. We compare our data to the Wigner surmise for Gaussian Unitary Ensemble (GUE), which is given by $P(s) = \frac{32}{\pi^2} s^2 e^{-4s^2/\pi}$, shown as dotted lines in Fig. 2.5. For small values of s , the bulk eigenmodes exhibit a quadratic level repulsion in agreement with the GUE prediction. However, at higher temperatures the data for the finer lattice corresponding to $N_\tau = 12$ do not agree very well with the GUE prediction for $s > 1$. The match remains reasonably good for small spacings $s < 1$. This mismatch can be attributed to

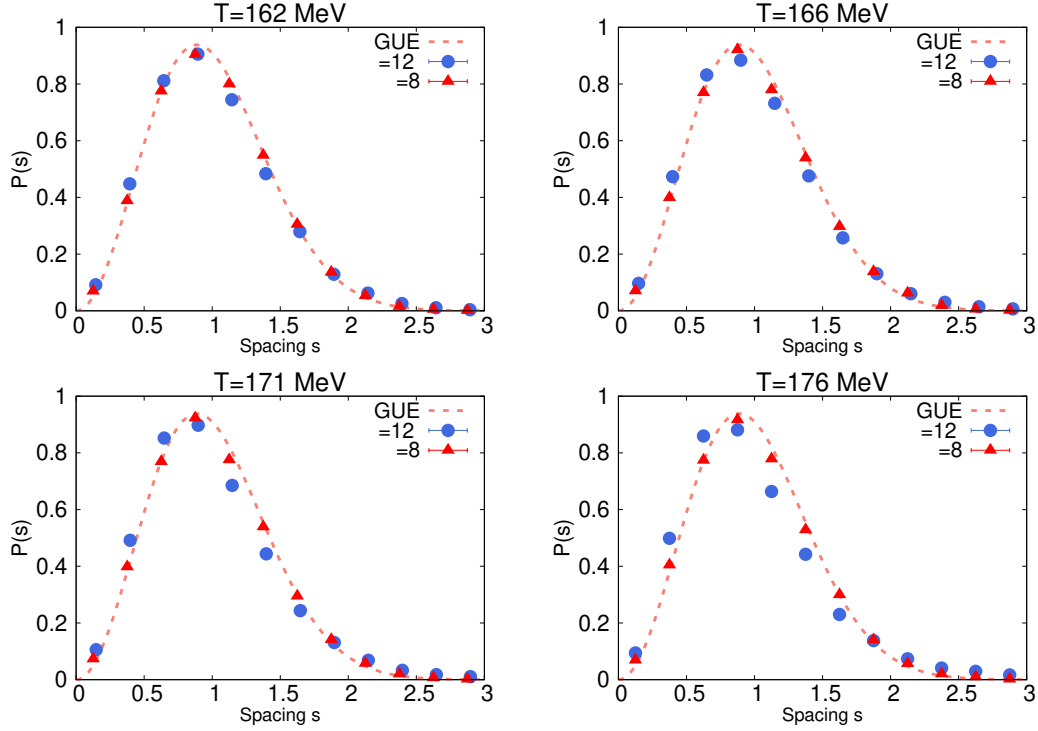


Figure 2.5: Unfolded level spacing distributions of bulk eigenmodes for different temperatures shown as a function of different lattice spacings or equivalently, N_τ . The dotted curves in each plot correspond to the Wigner surmise for Gaussian unitary random matrix ensembles.

the emergence of a near-zero peak-like pileup which overlaps with the bulk eigenmodes. On the finest $N_\tau = 16$ lattice, the near-zero peak-like formation is much more distinct at $T \geq 166$ MeV, see Fig. 2.1, hence the contamination is even stronger. As a result, the tail of the spacing distribution does not match with the GUE prediction at all.

To account for the long tail in the distributions, we use a fit ansatz given as $P(s) \sim s^2 \exp(-\alpha s)$. This function still has the correct quadratic repulsion at small s , but it falls off more slowly at larger s , the rate being controlled by the parameter α . Fitting our data with this function, we obtain values of $\alpha = 3.02(7), 3.17(9)$, and $3.3(1)$ respectively for temperatures $T = 162, 166$, and 171 MeV. As seen in Fig. 2.6, this ansatz function fits the $N_\tau = 16$ data very well for all temperatures above T_{pc} . This form of $P(s)$ is characteristic of a strongly interacting disordered system [100] where the universal level fluctuations of the eigenmodes deep in the bulk can be described in terms of RMT belonging to GUE, but the tails of the distribution show a different dependence. We will explore the physical

consequences of this mixing in the subsequent sections.

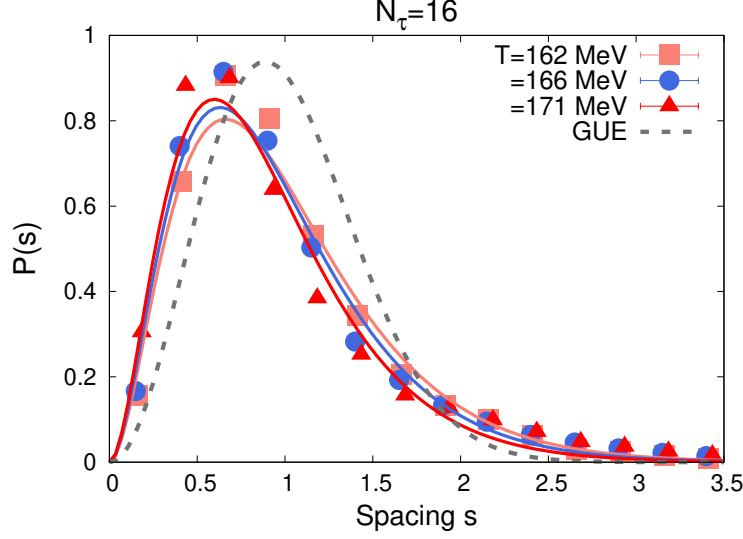


Figure 2.6: A fit to the eigenvalue level spacing distribution using a mixed ansatz for $N_\tau = 16$ at $T = 162, 166, 171$ MeV and compared with the prediction from a GUE of random matrices.

2.4 The fate of $U_A(1)$ breaking in the continuum limit

Because the flavor-singlet $U_A(1)$ symmetry is anomalous and hence lacks an order parameter, the magnitude of its breaking can be monitored from the difference in magnitude of the integrated meson correlators, $\chi_\pi - \chi_\delta$ [101]. In continuum, the relevant integrated meson correlators for $N_f = 2$ QCD are defined as,

$$\chi_\sigma = \int d^4x \langle \bar{\sigma}(x) \sigma(0) \rangle \quad (2.6)$$

$$\chi_\delta = \int d^4x \langle \bar{\delta}^i(x) \delta^i(0) \rangle \quad (2.7)$$

$$\chi_\eta = \int d^4x \langle \bar{\eta}(x) \eta(0) \rangle \quad (2.8)$$

$$\chi_\pi = \int d^4x \langle \bar{\pi}^i(x) \pi^i(0) \rangle, \quad (2.9)$$

with $i = 1, 2, 3$. The meson operators $\sigma(x) = \bar{\psi}(x) \psi(x)$ and $\delta^i(x) = \bar{\psi}(x) \tau^i \psi(x)$ denote the scalar isosinglet and scalar isotriplet states respectively and $\eta(x) = i\bar{\psi}(x) \gamma^5 \psi(x)$ and

$\pi^i(x) = i\bar{\psi}(x)\tau^i\gamma^5\psi(x)$ denote the pseudo-scalar isosinglet and pseudo-scalar isotriplet states, respectively. Here ψ represents the field operator corresponding to light quark doublet, and τ represents the isospin operator which are the Pauli matrices normalized by a factor of half. The above integrated correlators can further be written in terms of the connected and disconnected contributions as, $\chi_\sigma = \chi_{\text{disc}} - \chi_{\text{con}}$, $\chi_\delta = -\chi_{\text{con}}$, $\chi_\eta = -\chi_{\text{disc}}^5 + \chi_{\text{con}}^5$ and $\chi_\pi = \chi_{\text{con}}^5$. The $\text{SU}_A(2)$ restoration will lead to the relations $\chi_\delta = \chi_\sigma - \chi_{\text{disc}}$ and $\chi_\pi = \chi_\eta + \chi_{\text{disc}}^5$. The transformation properties among the meson multiplets under different subgroups of chiral symmetry are summarized in Fig. 2.7.

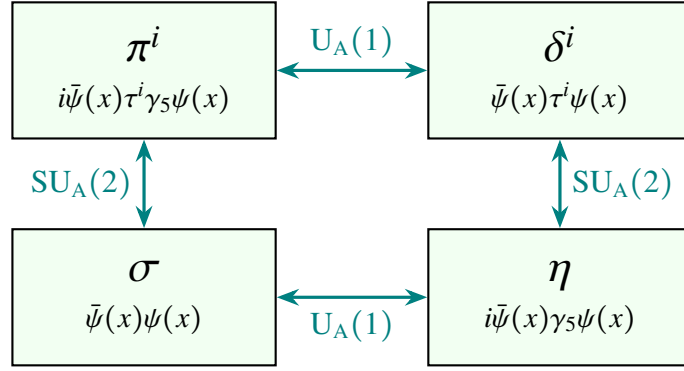


Figure 2.7: Under the $\text{SU}_A(2)$ transformation π^i and σ similarly δ^i and η form chiral multiplets which are represented by double arrows. The multiplets under $\text{U}_A(1)$ transformation are shown similarly.

To assess the breaking of the anomalous $\text{U}_A(1)$ symmetry, we calculate the dimensionless difference $(\chi_\pi - \chi_\delta)/T^2$ in terms of the eigenvalue of the massless Dirac operator written as $\int \frac{\rho(\lambda)}{T^2} \frac{4m^2}{(\lambda^2 + m^2)^2} d\lambda$ at all temperatures $T > T_{pc}$ and perform a $\sim 1/N_\tau^2$ continuum extrapolation, as illustrated in Fig. 2.8.

For the highest temperature $T = 176$ MeV, where only $N_\tau = 8$ and 12 data are available, the continuum estimate is assigned 40% and 20% uncertainties to the slope and intercept respectively, similar to the error estimates obtained after performing a continuum extrapolation at $T = 171$ MeV. We also observe that for our finest $N_\tau = 16$ lattice, about 99% of the magnitude of $(\chi_\pi - \chi_\delta)/T^2$ is due to near-zero eigenvalues. It is also evident from the figure that extrapolating the data from only the two finest lattices $N_\tau = 12, 16$ yields higher values of $(\chi_\pi - \chi_\delta)/T^2$ than from fits incorporating all three spacings. This

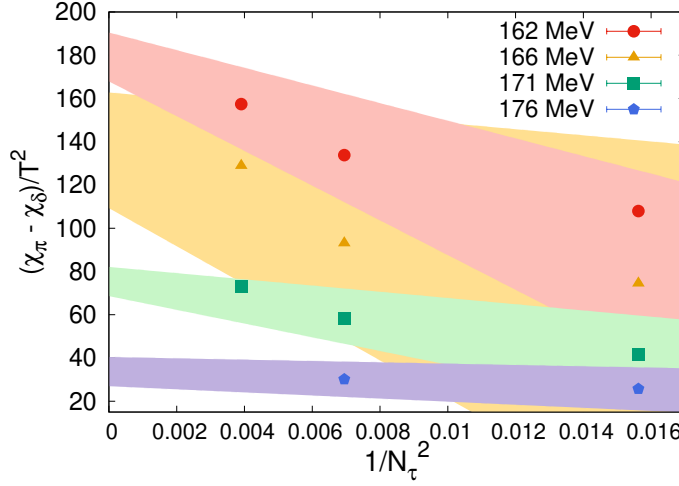


Figure 2.8: The continuum estimates for $\chi_\pi - \chi_\delta$ normalized by the square of temperature for HISQ fermions from three different lattice spacings corresponding to $N_\tau = 8, 12, 16$ at $T = 162, 166, 171$ MeV respectively and from $N_\tau = 12, 16$ data at $T = 176$ MeV.

confirms that non-zero values of this observable at $T > T_{pc}$ is exceptionally robust and thus the anomalous $U_A(1)$ symmetry is not effectively restored exactly at T_{pc} . Motivated from the facts that near-zero eigenmodes overwhelmingly contribute to $(\chi_\pi - \chi_\delta)/T^2$ and chiral perturbation theory predicts a characteristic $1/T^2$ dependence of this quantity [102] at $T \gtrsim T_{pc}$, we fit the continuum-extrapolated intercept values of the bands shown in Fig. 2.8 to the functional form $a + b/T^2$. As shown in Fig. 2.9, this fit allows us to extract the temperature $T/T_{pc} = 1.147(25)$ at which the dominantly large $1/T^2$ contribution to $U_A(1)$ -breaking observable vanishes.

It is interesting to remark here that the effective restoration of $U_A(1)$ was reported at a slightly higher temperature $T \sim 200$ MeV from the observation of degeneracy between (integrated) screening correlators $(\chi_\pi - \chi_\delta)/T^2$ in 2 + 1 flavor QCD using HISQ discretization [103] with a heavier than physical u,d-quark mass, corresponding to $m_\pi = 160$ MeV. The corresponding pseudo-critical temperature is also higher by ~ 4 MeV, hence the effective restoration occurs at $T \simeq 1.2 T_{pc}$, which is close to our estimates. Furthermore, a recent work [81] has reported breaking of $U_A(1)$ due to an $m^2\delta(\lambda)$ feature in the eigenvalue spectrum at about $1.5 T_{pc}$ which survives even in the chiral limit. We note here that

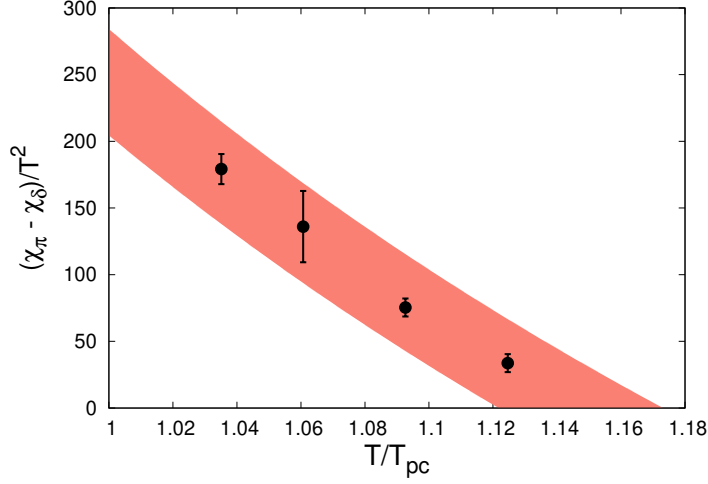


Figure 2.9: The continuum estimates for $(\chi_\pi - \chi_\delta)/T^2$ for temperatures greater than T_{pc} shown as points fitted to a functional form $a + b/T^2$ shown as a band.

$U_A(1)$ breaking due to this specific feature of the Dirac spectrum is expected to survive even at asymptotically high temperatures where the QCD vacuum can be explained in terms of a dilute gas of instantons [59, 61]. This is an inherent feature of an anomalous symmetry. Our analysis shows that a major, non-trivial breaking of the anomalous $U_A(1)$ subgroup of chiral symmetry arises due to the near-zero peak in the infrared part of the eigenvalue spectrum, which is quite different due to the breaking due to a dilute instanton gas. We show that this specific non-trivial contribution gets restored around $1.15 T_{pc}$, resulting in the opening up of a gap in the infrared part of the Dirac eigendensity profile with a small pile-up at $\lambda \rightarrow 0$ as reported in Ref. [81] that gives rise to a $\sim T^{-8}$ dependence for the topological susceptibility [59].

2.5 How well is the chiral Ward identity satisfied?

It is important to ensure that the (almost exact) 2-flavor chiral symmetry in QCD is recovered upon performing a continuum extrapolation of the relevant observables calculated on the lattice using HISQ discretization. We thus examine how well the chiral Ward identity is realized in the chirally symmetric phase. Restoration of the non-singlet subgroup of

2-flavor chiral symmetry requires that $\chi_\sigma = \chi_\pi$ and $\chi_\delta = \chi_\eta$, see Fig. 2.7. Consequently, the difference between integrated meson correlators can be written as $(\chi_\pi - \chi_\delta)/4 = \chi_{\text{disc}}^5$ [104], where the factor of 1/4 accounts for the four-fold taste degeneracy of the eigenspectrum of the HISQ Dirac operator in continuum. Furthermore, chiral Ward identity ensures that the disconnected chiral susceptibility is related to the topological susceptibility of QCD vacuum χ_{top} according to the relation $\chi_{\text{disc}}^5 = \chi_{\text{top}}/m^2$. We have calculated the values of $(\chi_\pi - \chi_\delta)m^2/T^4$ at each temperature using the HISQ Dirac eigenvalues at different lattice spacing and then performing a continuum extrapolation. The data for continuum extrapolated values of χ_{top}/T^4 were taken from Ref. [105].

A comparison between the continuum extrapolated values of χ_{top} and $\chi_\delta = \chi_\eta$ is presented in Fig. 2.10. The figure clearly demonstrates that for temperatures $T > 1.05 T_{pc}$, where the non-singlet subgroup of chiral symmetry is restored, the two quantities agree very well with each other within statistical errors. This agreement reassures that we indeed recover the chiral symmetry in QCD at $T > T_{pc}$ upon continuum extrapolation of the HISQ data.

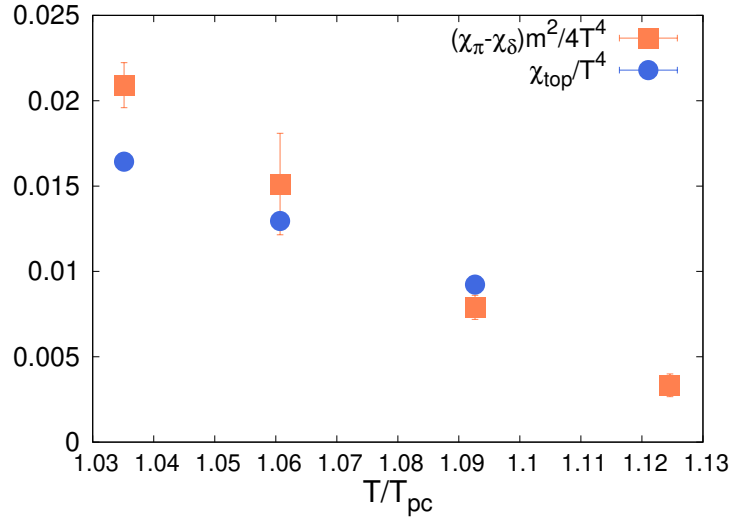


Figure 2.10: A comparison of the integrated renormalized correlator $\frac{m^2(\chi_\pi - \chi_\delta)}{4T^4}$ with the topological susceptibility (measured independently using gradient flow in Ref. [105]) for temperatures $> T_{pc}$.

2.6 Understanding $U_A(1)$ breaking in terms of the Dirac eigenspectrum

Having identified the properties of the near-zero and bulk eigenmodes, we will now understand the effective restoration of $U_A(1)$ in terms of these distinct features of the Dirac eigenspectrum.

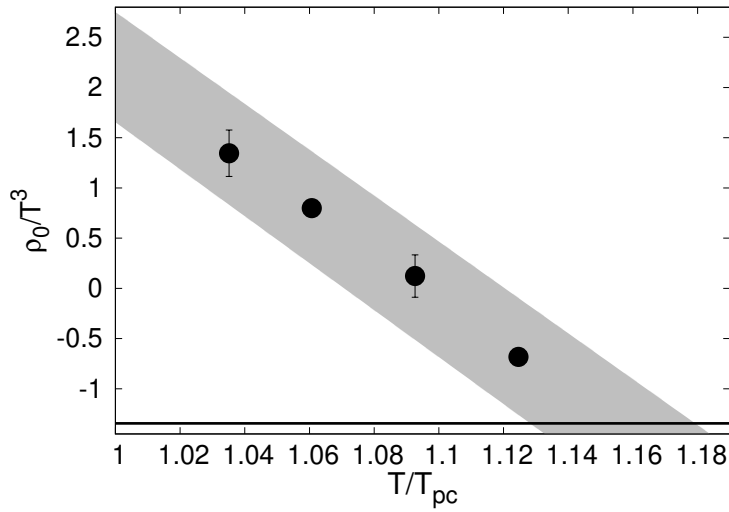


Figure 2.11: Continuum extrapolation of the bulk intercept for eigenvalue densities at different temperatures above T_{pc} . The horizontal line corresponds to $\rho_0/T^3 = -1.34$ for the bulk spectrum when it completely separates from near-zero eigenmodes.

First we determine the temperature at which the bulk eigenmodes fully separate from the peak-like feature due to the near-zero eigenmodes. Using the Dirac eigendensity calculated on the finest $N_\tau = 16$ lattice where the near-zero peak is clearly visible, we subtract the linear contribution due to the bulk eigenmodes from it. We observe that the near-zero peak has a typical width of $\lambda/T = 0.08$ across all temperatures above T_{pc} . Next we utilize the information about the continuum extrapolated slope $c_1/T^2 = 16.8(4)$, of the bulk eigendensity calculated earlier. For the near-zero and bulk eigenmodes to fully disentangle, the bulk eigendensity must drop exactly to zero where the near-zero start to pile up, which is around $\lambda/T = 0.08$. Based on the fact that bulk eigendensity grows linearly with λ , this

criterion requires that the intercept of the bulk eigenmodes is negative at $\lambda = 0$ when they disentangle from the near-zero eigenmodes. Using all these information in the fit function, one obtains an intercept $\rho_0/T^3 = -1.34$ for the bulk eigenmodes in the continuum limit, when they are separated from the near-zero eigenmodes.

Next we take the intercept of the eigenvalue density $\rho(\lambda)/T^3$ vs λ/T at each temperature $T > T_{pc}$ from Table 2.2 and obtain their continuum extrapolated values using the ansatz $\rho_0/T^3 + d/N_\tau^2$. At the highest temperature $T = 176$ MeV where only two data points are available, a conservative systematic error of $\sim 10\%$ is assigned to the extrapolated intercept. The resulting continuum extrapolated data for ρ_0/T^3 are shown in Fig. 2.11. Clearly, the values of ρ_0/T^3 decrease with increasing temperatures. Using a linear parameterization $\rho_0/T^3 = d_1(T/T_{pc}) + d_2$ to describe and fit this trend we obtain $d_1 = -23.1(3)$ and $d_2 = 25.3(3)$. Now we can ask the question, at what temperature is the intercept value $\rho_0/T^3 = -1.34$? Solving using the linear parametrization of ρ_0/T^3 as a function of temperature gives us $T = 1.15(3) T_{pc}$. Strikingly, this temperature estimate coincides with the effective restoration of $U_A(1)$ discussed in Section 2.4.

2.7 Summary and outlook

In this chapter, we addressed the long-standing question of whether the flavor-singlet $U_A(1)$ subgroup of the chiral symmetry is effectively restored simultaneously with the non-singlet subgroup in $2 + 1$ flavor QCD with a staggered discretization for quarks. By systematically performing a continuum extrapolation of the staggered (HISQ) Dirac eigenspectrum, we explicitly demonstrated that a non-trivial breaking of the anomalous $U_A(1)$ symmetry is a non-perturbative phenomenon governed entirely by the near-zero eigenmodes. Crucially, our continuum extrapolated results for $(\chi_\pi - \chi_\delta)/T^2$ which quantifies $U_A(1)$ breaking demonstrate a non-trivial breaking due to a $\sim 1/T^2$ term that persists up to $T \sim 1.15 T_{pc}$.

One can interpret the different (effective) restoration temperatures for different subgroups of chiral symmetry in terms of a more microscopic description in terms of instantons. Below T_{pc} , instantons are very closely situated and strongly correlated which is reflected in the strong repulsion between infrared eigenvalues consistent with a GUE of RMT. In the chiral symmetry restored phase however these strong long-range correlations weaken into a more liquid-like interaction among instantons [106]. This results in the near-zero eigenvalues piling up, forming a peak-like structure distinct from the bulk eigenmodes whose properties are consistent with those predicted in a GUE.

As temperatures increase further toward $T \sim 1.15 T_{pc}$, thermal screening severely suppresses these inter-instanton interactions [63, 107, 108]. This results in the reduction of the height of the near-zero peak-like feature. Consequently, the near-zero eigenmodes decouple and completely separate from the delocalized bulk spectrum. We demonstrate for the first time that this non-trivial spectral disentanglement and the subsequent vanishing of the near-zero peak leads to the effective restoration of $U_A(1)$ to its magnitude as predicted from a dilute gas model of instantons [109]. Interestingly, a separation between localized and extended Hamiltonian states strongly parallels the many-body localization transition in interacting electron systems in the presence of disorder [100].

It is important to note that the full restoration of an anomalous symmetry e.g., $U_A(1)$ symmetry, is never possible and manifests itself in a small residual breaking that can be understood in terms of a dilute instanton gas leading to a $\sim T^{-8}$ dependence of the topological susceptibility [59, 83]. Our study is based on a careful continuum extrapolation of the relevant physical observables, and hence our results are quite robust to systematic effects due to lattice discretization. Nevertheless, it will be important to verify these results by performing a study with Dirac operators that respect exact chiral symmetry on a finite lattice, which will be the topic of the subsequent chapters.

Chapter 3

Dynamical 2 + 1-flavor QCD with domain wall fermions and topology

3.1 Introduction

Simulating QCD at the physical point, set by the experimentally measured values of the pion and kaon masses, $m_\pi \approx 135$ MeV and $m_K \approx 495$ MeV, comes with a formidable computational cost. The Domain wall fermion (DWF) discretization provides a robust framework to preserve the almost exact two-flavor chiral symmetry of continuum QCD at a finite lattice spacing by introducing an auxiliary fifth dimension of extent L_5 . In principle L_5 has to be infinitely large to realize the chiral symmetry exactly. However for the simulations to be computationally viable, we use the Möbius domain wall fermion (MDWF) discretization for quarks. As motivated in the introductory Chapter 1, tuning additional *irrelevant* parameters in the MDWF allows one to reduce chiral symmetry violations for reasonably small values of L_5 thus providing a speed-up in the numerical code. Chiral symmetry violation which is quantified by the residual mass m_{res} is an order of magnitude smaller for MDWF at modest L_5 compared to the standard Shamir DWF action.

Despite this advantage there could be other practical challenges. One has to address the critical slowing down of Monte-Carlo algorithms near the chiral crossover transition. Typically molecular dynamics algorithms and its variants are better adapted to address this issue. Since the MDWF operator respects chiral symmetry to a good extent on the lattice, it will have significantly large number of infinitesimal eigenvalues. As a consequence, a slowing down of the hybrid molecular dynamics based algorithm will occur. Furthermore, simulations are typically performed on relatively coarser lattice spacings. Away from the continuum limit there could be unphysical localized gauge configurations which contribute to m_{res} making it larger than the mass of the light quarks. Such gauge configurations give rise to spurious near-zero modes that make the light quark determinant small enough to slow down the Monte-Carlo evolution. There are different techniques discussed in the literature to suppress these spurious zero modes on a finite lattice. Which of them will be more efficient for our problem of interest, namely the study of the chiral crossover transition with MDWF, needs a detailed investigation.

The primary discussion in this chapter revolves around optimization strategies for computing the light-quark determinant and for the nested multi-level integration scheme within the molecular dynamics algorithm to generate a large set of statistically independent thermal gauge configurations with MDWF. We show two important applications of the generated set of MDWF gauge ensembles. First we show that the restoration of the singlet and non-singlet subgroups of chiral symmetry does not occur at similar temperatures. We also study the temperature dependence of topological charge fluctuations using a probe overlap Dirac operator on these thermal MDWF gauge ensembles and compare with the earlier continuum extrapolated results obtained from a different fermion discretization.

3.2 Details of the numerical lattice calculations

In this work we have generated gauge configurations for $2 + 1$ -flavor QCD using the MDWF discretization for fermions and the Iwasaki gauge action for the gauge links. To remove localized dislocations in the gauge field, which contribute to the residual mass, we weighted the fermion determinant with the dislocation suppressing determinant ratio (DSDR) [110]. We performed simulations for a fixed lattice size, where the numbers of sites along the spatial and temporal directions were set to $N_s = 32$ and $N_\tau = 8$, respectively. The domain wall height was set to $M_5 = 1.8$. The light (m_ℓ) and strange (m_s) quark mass, the residual mass m_{res} , the extent of the fifth dimension L_5 and the Möbius parameters b_5 and c_5 were fixed following an earlier work using the same setup [11]. Unless mentioned otherwise all masses are in lattice units. The quark masses were fixed from simulations on zero temperature MDWF gauge configurations on two different bare values of the inverse gauge coupling $\beta = 6/g^2$ such that the pion mass is $129.2(5)$ MeV and the kaon mass is $462.5(5)$ MeV. The ratio of the strange to light quark mass $m_s/m_\ell \approx 27$ for all temperatures studied we have studied. The bare couplings are related to the lattice spacing using the 2-loop beta function in QCD. The temperatures $T = 1/(N_\tau a)$ can be calculated for each β and then expressed in physical units using the r_0 scale, following the earlier work [111]. The pseudo-critical temperature estimated using these sets of MDWF gauge ensembles is $T_{pc} = 158.7^{+2.6}_{-2.3}$ MeV [60].

We have also performed new optimizations within the hybrid Monte-Carlo (HMC) algorithm to achieve a speed-up in the generation of gauge configurations for this study which we will discuss in detail in the following sections. With these optimizations, the time required to generate each gauge configuration was reduced by approximately 20%, with a typical acceptance rate of about 90% for $T \lesssim T_{pc}$, and of more than 97% for $T > T_{pc}$. The gauge configurations were saved after every fifth HMC step of unit length to reduce the autocorrelation between the generated configurations. Whenever possible, we

combined in our analysis the datasets from the earlier analysis [11]. However the physical observables e.g. topological susceptibility were calculated on gauge configurations which are separated by 50-100 HMC steps in order to remove autocorrelation bias. The parameters used for the generation of gauge configurations, the studied temperature range and the number of MDWF configurations generated at each temperature are summarized in Table 3.1. We have estimated the residual mass on these configurations [60] and then combined it with the earlier results [111] for the same quantity, the outcome of which are also tabulated in Table 3.1.

T (MeV)	β	m_ℓ	m_s	b_5	N_{traj}	m_{res}
149	1.671	0.00034	0.05538	2.5	4875	0.00175(1)
154	1.689	0.00075	0.05376	2.5	3805	0.00120(1)
159	1.707	0.00112	0.05230	2.5	12520	0.00090(1)
164	1.725	0.00120	0.05045	2.5	6085	0.00068(1)
168	1.740	0.00126	0.04907	2.2	5160	0.00057(1)
177	1.771	0.00132	0.04614	2.0	6320	0.00043(1)
186	1.801	0.00133	0.04345	2.0	5920	0.00026(1)
195	1.829	0.00131	0.04122	1.9	2200	0.00019(1)

Table 3.1: Input parameters and generated gauge configurations on $32^3 \times 8$ lattices using the MDWF action. For all β values, the extent of the fifth dimension was fixed to $L_5 = 16$, the domain wall height to $M_5 = 1.8$, and the second Möbius parameter was set to $c_5 = b_5 - 1$. The table also reports the number of equilibrated trajectories after thermalization and the residual mass m_{res} estimated on the total number of configurations.

We also compare results for the topological susceptibility obtained on gauge ensembles generated using the MDWF action to corresponding results obtained with the HISQ action taken from Ref. [59]. The latter have been obtained by performing calculations on $2 + 1$ -flavor QCD configurations which were generated by the HotQCD collaboration in earlier studies [12] using the HISQ action and the tree-level improved Symanzik gauge action. The quark masses have been fixed for a physical strange-to-light quark mass ratio of $m_s/m_\ell = 20$. The lattice sizes used correspond to $N_\tau = 8, 12, 16$ and the number of spatial sites are $N_\sigma = 4 N_\tau$. We will use the jackknife resampling method to remove autocorrelation bias in the topological susceptibility calculated on the MDWF gauge configurations. Further details of the calculation of other observables e.g. the disconnected part of the

chiral susceptibility can be found in our published work [60] and in the thesis of Mischa Jaensch [112]. Our configuration generation codes were developed in part using the Grid Python Toolkit (GPT) [113] which uses the Grid library [114].

3.3 Algorithmic framework

In this section we will discuss about the details related to the generation of statistically independent gauge configurations in terms of $SU(3)$ valued gauge links $U_\mu(n)$ in $2 + 1$ -flavor QCD using the MDWF operator $D(U, m_s(m_\ell))$ for strange (light) quark flavor and Iwasaki gauge action $S_G(U)$ for the gluons [115]. We will sometimes not explicitly write the index μ in the gauge links. Here n denotes the lattice site. The fundamental quantity of interest is the QCD partition function,

$$\mathcal{Z} = \text{Tr} e^{-H_{\text{QCD}}/T} = \int \mathcal{D}(U) \det [D^\dagger(U, m_\ell) D(U, m_\ell)] \det [D(U, m_s)] e^{-S_G(U)}. \quad (3.1)$$

which is simply a path-integral over the configuration space of gauge links U_μ distributed according to the Boltzmann weight which is the product of the quark determinants multiplied with e^{-S_G} . We will be using the MDWF Dirac operator D for our study, which is defined as $\det D \equiv \frac{\det D(m_f)}{\det D(1)}$. The matrix elements of the 5D operator $D(m_f)$ are written as,

$$\begin{aligned} D_{s,s'}(m_f) = & (b_5 D_W + 1) \delta_{s,s'} \\ & + (1 - \delta_{s,1}) (c_5 D_W - 1) P_+ \delta_{s-1,s'} + (1 - \delta_{s,L_5}) (c_5 D_W - 1) P_- \delta_{s+1,s'} \\ & - m_f \delta_{s,1} (c_5 D_W - 1) P_+ \delta_{L_5,s'} - m_f \delta_{s,L_5} (c_5 D_W - 1) P_- \delta_{1,s'}, \end{aligned} \quad (3.2)$$

for mass m_f of quark flavor f . The indices $s, s' = 1, 2, \dots, L_5$, and $P_\pm = \frac{1 \pm \gamma_5}{2}$ are the left- and right-chiral projection operators. Here $D_W \equiv D_W(-M_5)$ denotes the 4D Wilson Dirac operator containing a domain-wall height parameter M_5 . The Möbius parameters b_5 and c_5 are tuned to reduce chiral symmetry breaking at fixed L_5 . The details of the parameters

used for the generation of thermal gauge configurations are mentioned in Table 3.1.

3.3.1 Hybrid molecular dynamics algorithm

Due to the high dimensionality of the configuration space and the non-local nature of the fermion determinant, traditional algorithms based on local updates of the gauge links become highly inefficient. To overcome this, it is economical to perform a molecular dynamics (MD) evolution in terms of a fictitious Hamiltonian but now defined in four dimensions [53] in terms of gauge fields that act as generalized coordinates and fictitious conjugate momenta.

Because the gauge links U are elements of the $SU(3)$ group, their conjugate momenta P must take values in the corresponding $su(3)$ Lie algebra. Thus, the fictitious momentum fields are written in terms of eight traceless, Hermitian generators T_i of the gauge group $SU(3)$ as

$$P_\mu(n) = \sum_{i=1}^8 P_\mu^i(n) T_i.$$

The numbers $P_\mu^i(n)$ are drawn independently from a Gaussian distribution $e^{-\text{tr}[P^2]}$ at the start of the MD evolution, where the kinetic energy $T(P)$ is denoted [53] as

$$\frac{1}{2} \sum_{n,\mu,i} \left(P_\mu^i(n) \right)^2 = \sum_{n,\mu} \text{tr} \left[P_\mu(n)^2 \right].$$

The light degrees of freedom are integrated out analytically to yield the quark determinant $\det [D^\dagger(U, m_\ell) D(U, m_\ell)]$. Introducing complex-valued, bosonic auxiliary fields known as pseudofermions, ϕ , allows one to rewrite the determinant in terms of an effective action $S_{\text{pf}}(U) = \phi^\dagger (DD^\dagger)^{-1} \phi$ as

$$\det [DD^\dagger] = \int \mathcal{D}\phi^\dagger(n) \int \mathcal{D}\phi(n) e^{-S_{\text{pf}}}. \quad (3.3)$$

The pseudofermion fields ϕ should be sampled with a probability $e^{-\phi^\dagger (DD^\dagger)^{-1} \phi}$. In order to

do so we draw a random vector χ by independently sampling the real and imaginary parts of each component from a normalized Gaussian distribution with unit variance, $e^{-\chi^\dagger \chi}$ such that $\phi(n) = D(U)_{n,n'} \chi(n')$.

While standard HMC efficiently simulates a pair of degenerate light quarks using the pseudofermion trick, this cannot be directly applied to the heavier strange quark flavor. Simulating a single strange quark flavor requires evaluating

$$\det [D(U, m_s)] = \det [D^\dagger(U, m_s) D(U, m_s)]^{1/2}.$$

Because this involves a fractional power of a positive definite operator, one can represent it in terms of rational function of such matrix operator. One can then use the multi-shift conjugate gradient for calculating the inverse of $D^\dagger(U, m_s) D(U, m_s)$ for constructing the rational polynomial. But due to the additional linear algebra operations associated with multi-shift conjugate gradient and the MD pseudofermion force make single flavor RHMC simulations relatively more costly than degenerate two flavor HMC simulations for the same bare quark mass. In our case we utilize the exact one flavor algorithm (EOFA) for strange quarks, which avoids the need for rational approximation of the strange quark determinant [116, 117]. The key to implement this technique is the observation that the ratio of fermion determinants can be factorized as a product of the inverse of two determinants, each of which involves an operator which is Hermitian and positive-definite [117]. Moreover it is possible to factorize the Möbius DWF operator $D = D_{\text{EOFA}} \tilde{D}$, into a one flavor operator D_{EOFA} which contains the gauge interactions, and a trivial identity operator $\tilde{D}$ that depends only on the Möbius parameters, L_5 and the quark mass. To summarize the ratio of determinants of a (Möbius) domain wall Dirac operators for two different mass parameters m_1 and m_2 can be written as

$$\det \left(\frac{D(m_1)}{D(m_2)} \right) \approx \det \left(\frac{D_{\text{EOFA}}(m_1)}{D_{\text{EOFA}}(m_2)} \right) = \int \mathcal{D}\phi_s^\dagger(n) \int \mathcal{D}\phi_s(n) e^{-\phi_s^\dagger \mathcal{M}_{\text{EOFA}} \phi_s}. \quad (3.4)$$

where $\mathcal{M}_{\text{EOFA}}$ is a Hermitian positive definite operator. Here $m_1 = m_s$ and $m_2 = 1$. This is an exact relation and allows one to avoid the truncation errors associated with a rational polynomial approximation. During the MD evolution, the EOFA offers significant computational advantages since inversions of the Dirac operator can be performed using the ordinary conjugate gradient algorithm rather than the multi-shift version required for rational hybrid MD. This substantially reduces the memory requirement while performing linear algebra with large matrices. For further details on EOFA, please refer to Ref. [117].

During the start of the MD evolution, we draw pseudofermion fields ϕ_s with a probability $e^{-\phi_s^\dagger \mathcal{M}_{\text{EOFA}} \phi_s}$. We re-use the Gaussian random vectors, χ already generated and then compute $\phi_s = \mathcal{M}_{\text{EOFA}}^{-1/2} \chi$. We then approximate the inverse square root by an appropriately constructed rational function, but note that this rational approximation enters only at the beginning of the MD evolution and is not necessary to compute the EOFA action itself or the associated pseudofermion force required during the MD.

The complete fictitious four dimensional Hamiltonian describing the gauge and pseudofermion fields can be compactly summarized as,

$$\mathcal{H}(U, P, \phi) = \sum_{n, \mu} \text{tr}[P_\mu(n)^2] + S_G[U] + \sum_{n, n'} \left[\phi^\dagger(n) (DD^\dagger)^{-1}_{n, n'} \phi(n') + \phi_s^\dagger(n) (\mathcal{M}_{\text{EOFA}})_{n, n'} \phi_s(n') \right]. \quad (3.5)$$

The system is then evolved along a fictitious MD time τ via Hamilton's equations of motion,

$$\frac{dP_\mu}{d\tau} = -F_\mu[U, \phi]; \quad \frac{dU_\mu}{d\tau} = i P_\mu U_\mu. \quad (3.6)$$

Momentum fields are updated using the force fields $F_\mu[U, \phi]$ which is an element of the $su(3)$ algebra and denoted as

$$F_\mu[U, \phi] = \sum_{i=1}^8 T_i \nabla_\mu^{(i)} \left[S_G[U] + \phi^\dagger (DD^\dagger)^{-1} \phi + \phi_s^\dagger \mathcal{M}_{\text{EOFA}} \phi_s \right], \quad (3.7)$$

where $\nabla_\mu^{(i)}$ represents the standard Lie derivative. At $\tau = 0$, the gauge fields are chosen

using either a cold start, where each link is initialized as an identity matrix, or a hot start, where links are sampled randomly from the SU(3) Haar measure. In practice, the choice is guided by the proximity of the initial state to the expected equilibrium configuration at a given gauge coupling, with the cold start typically preferred for simulations in the weak-coupling regime. Alternatively, for continued Markov chains, the initial configuration is taken from a previously saved gauge link to bypass the thermalization phase. Regardless of the choice of U , the conjugate momenta P_μ are refreshed at the beginning of each trajectory by drawing from a Gaussian distribution, ensuring the system explores the phase space with the correct kinetic energy. The χ 's are held fixed during the subsequent MD evolution. To integrate the equations of motion given in Eq. 3.6 we employ a multi-scale, second-order Omelyan integrator [118]. This is a symplectic integrator and ensures time reversal invariance up to $\mathcal{O}(\delta\tau^2)$ where $\delta\tau$ denotes the discrete time-steps. Each infinitesimal update of the links and the conjugate momenta are represented as

$$\begin{aligned} T_U(\delta\tau) : \quad & U_\mu(n, \delta\tau) = e^{iP_\mu(0)\delta\tau} U_\mu(n, 0) \quad , \quad P_\mu(\delta\tau) = P_\mu(0) ; \\ T_P(\delta\tau) : \quad & U_\mu(n, \delta\tau) = U_\mu(n, 0) \quad , \quad P_\mu(\delta\tau) = P_\mu(0) - \delta\tau F_\mu . \end{aligned} \quad (3.8)$$

In terms of these infinitesimal updates the total time evolution operator T of the fields and momenta over a trajectory of length $\tau = N\delta\tau$ for the second-order Omelyan force-gradient integrator with a tunable parameter α is denoted as

$$T = \left[T_P(\alpha\delta\tau) T_U\left(\frac{\delta\tau}{2}\right) T_P(\delta\tau(1-2\alpha)) T_U\left(\frac{\delta\tau}{2}\right) T_P(\alpha\delta\tau) \right]^{\frac{N}{2}} . \quad (3.9)$$

The parameter α has been tuned to a value $1/6$ such that a significant gain in performance is achieved compared to the conventional leap-frog integrator [119]. To further optimize the computational cost, we employ a multi-timescale integration scheme where the gauge and fermion forces in Eq. 3.7 are evolved using different step sizes. For the gauge force, we typically use $N = 32-48$ integration steps, while for the computationally demanding fermion force $N = 8-12$ steps are used, maintaining the total trajectory length at $\tau = 1$.

Errors build up during the MD evolution since the integrator is not numerically exact resulting in the non-conservation of the Hamiltonian by an amount $\Delta\mathcal{H}$. This is corrected via a Metropolis accept/reject step. Thus in the so-called hybrid molecular dynamics algorithm the time evolved configuration is accepted with a probability $\min(1, e^{-\Delta\mathcal{H}})$, which exactly corrects for any numerical errors introduced by the choice of the integrator.

The CG iterations are performed in single precision to maximize memory bandwidth and computational throughput. Double-precision corrections are then applied at the end of the CG to guarantee tolerance of 10^{-10} . This level of accuracy is necessary to maintain the exact reversibility of the MD trajectory, thereby preventing large energy violations and ensuring a high acceptance rate in the final Metropolis accept/reject step.

3.3.2 Dislocation Suppressing Determinant Ratio (DSDR)

Domain wall fermions are designed to minimize chiral symmetry breaking even on a finite lattice spacing, quantified in terms of a residual mass m_{res} . The amount of explicit breaking of chiral symmetry depends on the fifth-dimensional extent of the lattice L_5 and is quantified through the expression [120],

$$m_{\text{res}} = \rho_H(\lambda_c) \frac{e^{-\lambda_c L_5}}{L_5} + \rho_H(0) \frac{1}{L_5}. \quad (3.10)$$

Here $\rho_H(\lambda)$ is the density of the eigenvalues λ of the effective 4D Hamiltonian matrix $H = -\log(\mathcal{T})$, where $\mathcal{T}$ denotes the transfer matrix that relates the quark fields on the adjacent four dimensional slices along the fifth direction. The $\rho_H(0)$ in the above expression denotes the density of near-zero modes and $\rho_H(\lambda_c)$ the density near the mobility edge λ_c that separates the near-zero from the delocalized bulk eigenfunctions. In the absence of gauge interactions or for sufficiently smooth gauge fields, a gap appears in the eigen-spectrum of H i.e., $\rho_H(0) \rightarrow 0$, resulting in the residual mass to decay exponentially with L_5 . However, when gauge couplings are non-perturbatively large and for coarser lattice

spacing which are typically the case for lattice studies at temperatures below or immediately about the crossover temperature, localized gauge field configurations of the size of the lattice spacing called dislocations, proliferate. These dislocations are unphysical UV configurations of rough gauge fields which give rise to near-zero eigenmodes thus augmenting the relative contribution of the $1/L_5$ term in m_{res} . One has to choose comparatively larger values of L_5 in order to keep the m_{res} to tolerable values thus increasing the computational cost.

To suppress these dislocations and increase the gap in the infrared eigenspectrum $\rho_H(\lambda)$ it was suggested [121] to introduce two flavors of heavy Wilson fermions with a negative mass of magnitude M_5 . These heavy quarks thus decouple in the continuum limit giving the correct QCD partition function. One can interpret these additional flavors to provide a fermion determinant that reweights the gauge action thereby suppressing unwanted rough gauge configurations. However it was realized that this numerical trick might also result in suppressing the physical topological tunneling in the gauge fields and giving unwanted effects in the ultraviolet region. Hence an improved version of this simple trick was suggested which leads to reweighting the gauge field action with the dislocation suppressing determinant ratio (DSDR). The DSDR [110] is constructed out of two degenerate heavy Wilson quark flavors with a small imaginary twist ϵ_f and additional two flavors of pseudo-fermions with equal mass $-M_5$ and an imaginary twisted mass ϵ_b to suppress the UV fluctuations [122], compactly summarized as

$$\mathcal{W}(M_5, \epsilon_b, \epsilon_f) = \frac{\det[D_W^\dagger(-M_5)D_W(-M_5) + \epsilon_f^2]}{\det[D_W^\dagger(-M_5)D_W(-M_5) + \epsilon_b^2]}. \quad (3.11)$$

Typically $0 < \epsilon_f \ll \epsilon_b < 1$. In our simulations, the DSDR is also implemented as a three-step ratio to ensure numerical stability and faster inversion. The three sets of $\{\epsilon_f, \epsilon_b\}$ we have chosen are $\{0.02, 0.07\}$, $\{0.07, 0.18\}$ and $\{0.18, 0.5\}$. This three-step ratio ensures that the residual mass m_{res} remains reasonably suppressed without compromising on physical topological tunneling due to instantons and the Metropolis acceptance rate.

3.4 Techniques to accelerate the HMC algorithm

Simulating QCD ensembles for light quarks at the physical point is computationally challenging due to the proliferation of very small eigenvalues of the Dirac operator, leading to very slow fermion updates in the molecular dynamics evolution. This in turn increases the time required to generate statistically independent gauge configurations. To make our simulations computationally viable, we have used two primary optimization strategies: Hasenbusch mass preconditioning with a careful tuning of an intermediate set of masses and optimizing the ratio of the number of fermion to gauge force integration steps per HMC trajectory.

3.4.1 Hasenbusch Preconditioning

Hasenbusch mass pre-conditioning [123] reduces the time required to compute the light-quark forces by splitting the fermion determinant into a product of ratios involving Dirac matrices with closely chosen mass parameters such that the condition number of these ratios are much lower compared to the condition number of the Dirac operator for the light quark. Choosing appropriate intermediate masses is a crucial step to optimize the most time-consuming step during the HMC evolution i.e., calculating light quark forces which involves inversion of the Dirac matrix. This is more so relevant for Möbius domain wall operator which has many near-zero eigenvalues at gauge couplings relevant for our study, due to which its inversion is computationally challenging. Furthermore, the presence of small eigenvalues leads to larger fermion forces, due to which one needs to decrease the step size $\delta\tau$ for the fermion integrator. This in turn leads to performing more frequent Dirac matrix inversions, which slows down the HMC algorithm.

To address this, n intermediate masses $m_1, m_2, \dots, m_n$ are introduced such that $m_\ell < m_1 < m_2 \dots m_n < 1$. Now implementing the Hasenbusch pre-conditioning with these intermedi-

ate masses [123] leads to the factorization of light quark determinant as,

$$\det \left(\frac{D^\dagger(m_\ell)D(m_\ell)}{D^\dagger(1)D(1)} \right) = \det \left(\frac{D^\dagger(m_\ell)D(m_\ell)}{D^\dagger(m_1)D(m_1)} \right) \det \left(\frac{D^\dagger(m_1)D(m_1)}{D^\dagger(m_2)D(m_2)} \right) \dots \det \left(\frac{D^\dagger(m_n)D(m_n)}{D^\dagger(1)D(1)} \right). \quad (3.12)$$

Each Hasenbusch ratio allows for splitting the original light fermion force term into manageable components with a smaller condition number such that it enters into the expression of $\mathcal{H}$ governing the MD evolution as,

$$-\sum_{i=0}^n \phi_i^\dagger D(m_i) \frac{1}{D^\dagger(m_{i-1})D(m_{i-1})} D^\dagger(m_i) \phi_i, \quad m_0 \equiv m_\ell. \quad (3.13)$$

The effectiveness of this preconditioning relies heavily on the precise tuning of the intermediate masses m_i . Because the L^∞ norm of the fermion force vector is correlated with the overall HMC acceptance ratio, the intermediate masses are carefully chosen to balance the fermion forces across all quotient actions [124]. Keeping the L^∞ norm of the quotient term containing the lightest quark mass slightly smaller than the others is often beneficial since we reduce the contribution of more expensive terms in the force [124]. This allows for choosing time steps based on the relative importance of the force contributions, thus optimizing the MD algorithm compared to the version without any mass preconditioning.

In our study, we use six Hasenbusch ratios with intermediate masses $\{0.006, 0.017, 0.07, 0.18, 0.45\}$ to optimize the light-quark force calculation in the generation of an extensive set of 2 + 1-flavor Möbius domain wall configurations. This setup provided further acceleration compared to the earlier implementation using five Hasenbusch ratios with intermediate masses $\{0.017, 0.07, 0.18, 0.45\}$. This ensures that the successive mass ratios are nearly the same i.e., $m_{i-1}/m_i \approx 0.4$, allowing for an optimal balance of the fermion force term. This made our code $\sim 4\text{-}25\%$ faster when going from $T = 159\text{-}186$ MeV, keeping the acceptance rates high enough $\sim 90\%$.

3.4.2 Tuning fermion and gauge force integration steps

To manage the vastly different magnitudes of the force terms due to gauge and fermion actions, a multiple time-scale integration scheme is implemented. This scheme exploits the fact that the gauge force term is computationally inexpensive but has large fluctuations, while the fermion force terms are computationally demanding but have a smaller magnitude. Consequently, the gauge fields have to be updated more frequently at finer MD time steps $\delta\tau$, while fermion force terms are integrated on a coarser time scales. This choice of multiple time-scales significantly reduces the total computational overhead.

Once the force term for the degenerate light quarks are factorized and optimized using Hasenbush pre-conditioning, an optimization of the number of integrations performed per HMC trajectory has to be done. We remind here that the total length of the HMC trajectory is kept fixed i.e., $\tau = 1$. At temperatures $T \lesssim T_{pc}$ we have reduced the number of integration steps for the gauge force term from previously used [111] 48 to 32 and performed fermion force updates 8 times per trajectory instead of previously used 12 times, keeping the average acceptance rate at $\gtrsim 80\%$. This made our HMC code faster by 20% – 25%. At a higher temperature $T = 186$ MeV we could achieve an even higher $\sim 40\%$ speed-up of our code by performing gauge and fermion updates 32 and 8 MD time steps respectively during a HMC evolution, keeping the acceptance rate at $\gtrsim 90\%$.

3.5 Results

3.5.1 Topological charge fluctuations

To ensure that the topology is properly sampled in the MDWF gauge configurations we have generated, we calculate the topological charge Q for gauge configurations separated by 50-20 hybrid Monte-Carlo trajectories. The Q is measured by counting the number

of exact zero eigenvalues of the overlap Dirac operator which are used as a probe for these gauge configurations. The overlap Dirac operator was numerically constructed such that on each configuration the Ginsparg-Wilson relation and the realization of the sign-function were implemented with a precision of $\lesssim 10^{-9}$. The overlap Dirac operator has an index [36] which is related to the topological features of the underlying gauge configurations if the gauge links are sufficiently smooth [42]. Furthermore since the overlap zero modes come with a definite chirality of either $+1$ or -1 , the overall sign of the total topological charge in each configuration is also known. We show the Monte-Carlo time history of the topological charge in each stream and for different temperatures we have studied in Fig. 3.1. It is thus clearly evident that the topology is not frozen during MC time evolution and all topological sectors are sampled optimally in the thermal gauge configurations. The average value of the topological charge measured on the available ensembles, $\langle Q \rangle \lesssim 10^{-2}$ for all temperatures we have studied, ensuring that the CP-even condition for QCD is maintained to a very good numerical precision. From the same figure, we also observe that large fluctuations of Q are suppressed at higher values of temperatures, consistent with the expectations that topological tunnelings should become rarer at higher temperatures.

Next, we compare how well the topological tunnelings that occur in QCD are represented in the gauge configurations generated using the HISQ and MDWF discretizations for fermions. This comparison is important for two reasons. First, for the domain-wall fermions, one can be assured that the topological tunnelings are adequately represented even at non-vanishing lattice spacing without any significant contributions arising from localized dislocations whose size is of the order of a single lattice spacing, quite unlike in the case for staggered fermions at a similar value of the lattice cutoff. Second, the domain-wall Dirac matrix violates continuum chiral symmetries through terms that are irrelevant in the continuum limit, unlike the HISQ discretization where the chiral symmetry group and hence the notion of an index is altered on a finite lattice due to rooting. It is not apriori clear what the consequences of this fact are for the topological suscept-

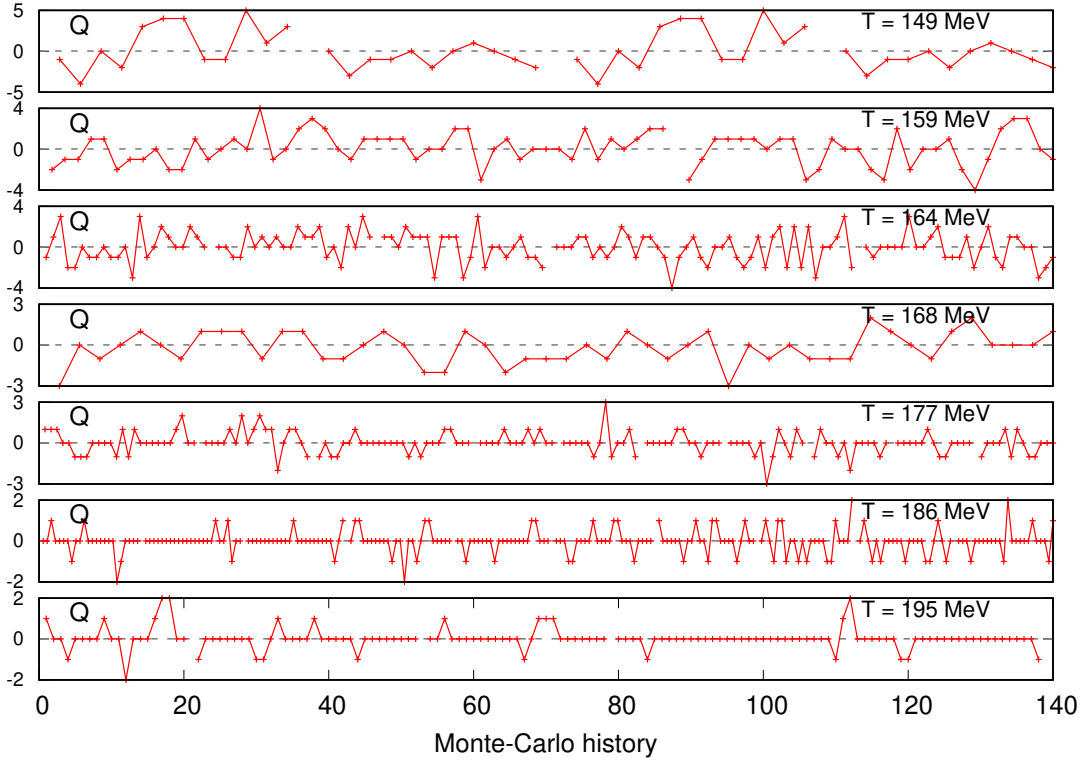


Figure 3.1: The Monte-Carlo time-history of the topological charge Q measured on independent gauge configurations at different temperatures used in this work. The x-axis shows the configuration number which is scaled at different temperatures for better visibility. The data points represent the value of topological charge Q at each configuration, which are typically separated by 50-20 HMC trajectories for temperature $T = 149$ -195 MeV. The gaps in the time-histories represent the start of different independent streams in the Monte-Carlo evolution.

ibility obtained using the HISQ discretization, i.e., how fine lattices would be required to perform a correct continuum extrapolation of this observable. In the literature, there have been extensive discussions on whether the topological fluctuations are correctly accounted for in rooted staggered fermions [125]. In the weak-coupling lattice perturbation theory it has been shown that a four flavor-taste staggered determinant factors into four equivalent determinants and that the correct flavor symmetries emerge in the continuum limit [126–129]. For staggered fermions, however, the flavor singlet subgroup of chiral symmetry which is sensitive to topology, has to be defined carefully on a finite lattice. Previous studies reconstructing the t’Hooft vertex and the flavor singlet meson correlator from the near-zero-mode quartets showed the emergence of the expected behavior

of these observables in the continuum [130] and more recently reproduced the η' meson mass using the staggered discretization of QCD in the continuum limit [131].

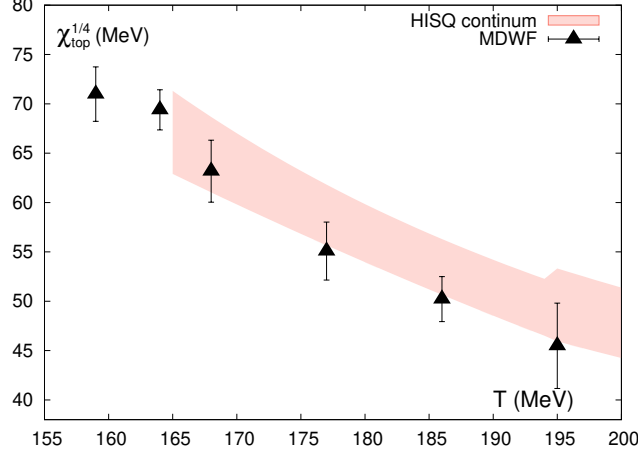


Figure 3.2: Comparison of $\chi_{\text{top}}^{1/4}$ (in MeV) between continuum extrapolated results using the HISQ discretization taken from Ref. [59] versus the values we have obtained in 2 + 1-flavor QCD using the MDWF discretization.

The fluctuations of the topological charge within a volume V and at a temperature T is measured in terms of the quantity $\chi_{\text{top}} = \frac{T}{V} \langle Q^2 \rangle$. The values of $\chi_{\text{top}}^{1/4}$ calculated on the gauge configurations generated with MDWF discretization on an $N_\tau = 8$ lattice is compared with corresponding continuum extrapolated values obtained by using the HISQ discretization from Ref. [59] in Fig. 3.2. The topological charge on the HISQ configurations was obtained using the improved clover definition, after performing Symanzik flow to reduce the ultra-violet noise resulting from gauge fluctuations [105]. We observe that, even though the results obtained from the MDWF ensembles are for a fixed lattice spacing, these are consistent with the continuum extrapolated results obtained using HISQ fermions. It is to be noted that the calculations involving MDWF consisted of $\mathcal{O}(10^2)$ i.e., only about a tenth of the configurations we have generated, whereas the HISQ results were obtained using $\mathcal{O}(10^3)$ configurations. Our results demonstrate a first comparison of the topological susceptibility, at finite temperature, of continuum extrapolated HISQ results with MDWF, highlighting the importance of improved realization of chiral symmetry on the lattice also for a proper topological sampling among the gauge configurations.

3.5.2 Effective restoration of singlet and non-singlet subgroups of chiral symmetry

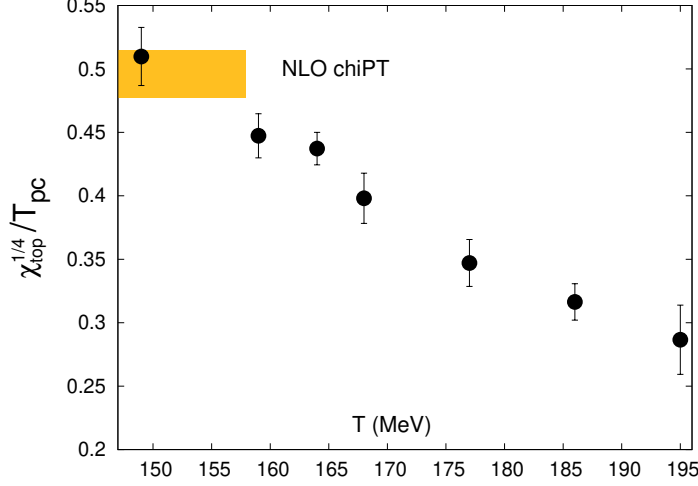


Figure 3.3: Topological susceptibility $\chi_{\text{top}}^{1/4}/T_{pc}$ (circles) calculated in 2 + 1-flavor QCD with MDWF discretization on an $N_\tau = 8$ lattice compared to its values calculated in NLO SU(2) chiral perturbation theory (yellow band).

To understand the topological contribution to the breaking of different subgroups of chiral symmetry, we estimate the temperature dependence of the topological susceptibility. It is known from an earlier study [102] using an improved version of staggered fermions that the χ_{top} in 2 + 1-flavor QCD is consistent with the prediction from next-to-leading order (NLO) chiral perturbation theory (chiPT),

$$\chi_{\text{chiPT}}^{\text{NLO}} = \frac{z}{(1+z)^2} M_\pi^2 F_\pi^2 [1 + \delta_1], \quad (3.14)$$

where $\delta_1 = \frac{2M_\pi}{F_\pi^2} (h_1^r - h_3^r - l_4^r - l_7)$ in terms of low energy constants of SU(2) chiral perturbation theory [132]. For our case, z , which is the ratio of mass of up and down quarks, is simply $z = 1$. Using the latest values of $F_\pi = 94.15 \text{ MeV}$, $M_\pi = 134.98 \text{ MeV}$ and the quantity $(h_1^r - h_3^r - l_4^r - l_7) = -0.0114$ from the FLAG review [133], we obtain the $(\chi_{\text{chiPT}}^{\text{NLO}})^{1/4} = 78.8 \pm 2.9 \text{ MeV}$, where the error predominantly comes in the determination of F_π . The contribution to the chiral observables from strange quarks is small compared

to the light quarks hence we consider two-flavor chiral perturbation theory. In Fig. 3.3 our results for $\chi_{\text{top}}^{1/4}/T_{pc}$, calculated in 2 + 1-flavor QCD using the MDWF discretization is shown as a function of temperature. For $T < T_{pc}$ our results for χ_{top} agree very well with the prediction from NLO chiPT. However on increasing temperatures $T \gtrsim T_{pc}$, the χ_{top} already starts to deviate from the chiPT prediction. This deviation widens with increasing temperatures, reaching an approximate 50% of the chiPT value at the highest temperature $T = 195 \text{ MeV}$. This shows that topological fluctuations already hint at the onset of a phase where chiral symmetry is gradually restored. The magnitude of χ_{top} slowly approaches $m_\ell^2 \chi_{\text{disc}}$ with increasing temperatures [60]. The details about the calculation of χ_{disc} and its comparison with χ_{top} are available in Mischa Jaensch's thesis [112]. Aside from a small deviation resulting from the finite mass of the light quarks, this convergence also signals the effective restoration of the non-singlet subgroup of the chiral symmetry.

Furthermore, the temperature dependence of our data for $\chi_{\text{top}}^{1/4}/T_{pc}$ at $160 < T < 186 \text{ MeV}$ can be characterized by a power law $(T/T_{pc})^{-\alpha}$ with an exponent of $\alpha = 2.4(2)$. A dilute instanton gas model [109] which represents fluctuations of isolated, uncorrelated instantons is expected to describe the QCD vacuum at asymptotically high temperatures. In this model the temperature dependence of topological susceptibility in QCD with two light quark flavors is described by an exponent of $\alpha \approx 2$. The fact that our extracted exponent is $\alpha > 2$ reflects a nontrivial breaking of the $U_A(1)$ symmetry up to $T_{pc} < T \lesssim 186 \text{ MeV}$, where the magnitude of χ_{top} is largely due to a finite strange quark condensate [134]. Since this dependence is unlikely to be explained by a dilute instanton gas-like scenario, it demonstrates that the singlet $U_A(1)$ part of the chiral symmetry is not yet *effectively* restored in this temperature regime. However higher statistics and continuum extrapolation for χ_{top} are required in order to accurately determine its temperature dependence.

3.6 Summary and outlook

In this chapter, we have shown the importance of the MDWF discretization for studying QCD near the chiral crossover and the challenges in its implementation. Since the light quark mass is significantly smaller than any other scales in finite temperature QCD, the two-flavor chiral symmetry is respected to a very good extent thus it is important to address the question of whether its singlet and non-singlet subgroups are (effectively) restored simultaneously. Addressing this question on the lattice using the more often used HISQ discretization is more subtle, since it breaks the non-singlet chiral symmetry group to a remnant $U(1)$ subgroup, as a result of a mixing between the spin and flavor degrees of freedom. Furthermore, due to the lack of an exact index of the HISQ Dirac matrix, the connection between topological fluctuations and the *effective* restoration of the $U_A(1)$ subgroup of chiral symmetry in QCD is not manifest. We have discussed how MDWF, which respects the chiral symmetry to a good extent on a finite lattice, can allow us to convincingly track the *effective* restoration of different subgroups of the almost exact chiral symmetry in QCD even on a finite lattice spacing.

Generating independent gauge ensembles using the MDWF brings its own challenges, which we discuss in detail in this chapter. I have also discussed some of the optimizations and improvisations that we have implemented to make our hybrid Monte-Carlo code numerically more efficient. As a result we could demonstrate [60], that the non-singlet subgroup of chiral symmetry is *effectively* restored at a pseudo-critical temperature $T_{pc} = 158.7^{+2.6}_{-2.3}$ MeV which is in very good agreement with the result of $T_{pc} = 156.5 \pm 1.5$ MeV obtained using HISQ discretization, but after performing a careful continuum extrapolation. The details of its extraction and discussion on the *effective* restoration of the non-singlet subgroup of chiral symmetry is one of the topics in the thesis by Mischa Jaensch [112]. In this chapter of my thesis, I mainly focused on the study of $\chi_{\text{top}}^{1/4}/T_{pc}$ and its implications for the singlet subgroup of chiral symmetry. Nevertheless the increasing

deviation of $\chi_{\text{top}}^{1/4}/T_{pc}$ values from its chiral perturbation theory prediction as a function of temperature can already hint towards *effective* restoration of the non-singlet subgroup of (almost exact) chiral symmetry in QCD.

Further we show that topological fluctuations of $N_\tau = 8$ MDWF gauge ensembles quantified by χ_{top} , are similar in magnitude to the continuum extrapolated values calculated on the HISQ gauge ensembles. This highlights once more the role of chiral symmetry in realizing the topological fluctuations more accurately. By determining the exponent controlling the temperature dependence of χ_{top} using MDWF calculations, we have shown that at $T \lesssim 185 \text{ MeV}$ the singlet subgroup of the chiral symmetry is not yet *effectively* restored, i.e., to its value at asymptotically high temperatures known within the dilute instanton gas approximation.

It would be important to study in detail the properties of the eigenvalues and eigenvectors [62, 65, 73, 111] of a lattice Dirac operator with good chiral properties on these MDWF gauge ensembles in order to better understand the mechanism underlying the restoration of different subgroups of chiral symmetry. This topic will be addressed in the next Chapter 4.

Chapter 4

The QCD Dirac eigenspectrum at finite temperatures using chiral fermions on the lattice

4.1 Introduction

We have discussed in Section 1.3 how the eigenvalue spectrum of the Dirac operator provides important insights regarding the symmetries of QCD and their breaking. The intercept of the near-zero eigenmodes of the Dirac operator in the chiral symmetry broken phase gives an accurate estimate of the chiral condensate, the order parameter of the chiral phase transition in the limit of massless quarks [54]. At higher temperatures, when the non-singlet subgroup of the almost exact two-flavor chiral symmetry is *effectively* restored, the intercept vanishes leading to the formation of a small peak-like feature in the infrared part of the eigenvalue spectrum. This peak has been observed in studies using a mixed-action set-up [61–63] which was debated for a while [64–67]. However, the existence of the peak was shown with dynamical domain wall fermions [68] on a finite lattice, now also observed to survive in the continuum limit in 2+1 QCD with HISQ

discretization [69] as detailed in Chapter 2.

The higher (bulk) eigenvalues λ whose density varies linearly with λ are disordered i.e., their level spacing ratios are consistent with the predictions from RMT belonging to the GUE. The peak-like feature and the linearly rising bulk spectra overlap strongly, resulting in eigenvectors which are delocalized [70–72] but not ergodic and whose level spacing fluctuations are *intermediate* between the Poissonian and GUE values [73]. Eventually the $U_A(1)$ subgroup will be also *effectively* restored at a temperature, $T_{U(1)}$, when physical observables which are sensitive to it, e.g., the topological susceptibility has a temperature dependence which is consistent with that expected from a dilute gas of instantons. We have obtained $T_{U(1)} \gtrsim 1.2 T_{pc}$ from the fact that the contributions in $\chi_\pi - \chi_\delta$ due to a near-zero peak-like feature of the infrared eigendensity vanishes at this temperature [69]. More stringent bounds on $T_{U(1)}$ are discussed in the literature. A $T_{U(1)} \gtrsim 1.5 T_{pc}$ is inferred from the temperature dependence of the topological susceptibility in QCD [59], from the features in the Dirac eigenvalue spectrum [61, 72], from the degeneracy of temporal meson correlators [77] and through tensor singlet channels [80].

The scenario at even higher temperatures $T > T_{U(1)}$ is not yet well understood. Whereas a peak-like feature of near-zero eigenmodes similar to $m^2\delta(\lambda)$ should survive, expected from a dilute gas-like scenario for instantons [61, 72, 81, 82], it is heavily suppressed as a function of temperature. Thus its contribution to topological susceptibility decreases as $\sim T^{-8}$ [59, 83, 84]. Eventually these infrared modes should be gapped out from the bulk part of the eigenvalue spectrum. Recent studies indicate that at sufficiently high temperatures, the most infrared part of this bulk spectrum contains localized eigenvalues which can be distinguished from the other delocalized bulk eigenmodes, which follow GUE level statistics, through a mobility edge [63, 85, 86]. This phenomenon is analogous to a localization transition [63, 86–91] observed in the Anderson model [92]. Nonetheless, a naive Anderson-like scaling of its temperature dependence demonstrates that the mobility edge might vanish at the pseudo-critical temperature [63, 87, 94], but it might also

disappear only at the critical temperature which is achieved in the chiral limit [86]. The robustness of these observations needs to be tested through carefully performed infinite volume and continuum extrapolations.

To summarize, whereas there is a wealth of results on spectral signatures related to *effective* restoration of the different subgroups of chiral symmetry, and on the localization properties akin to an Anderson-like transition, separately, the interplay between these two physically distinct phenomena is not so clear. We want to emphasize here that these two phenomena are of distinct physical origin and thus their consequences will also be different. Anderson transition is a quantum phase transition which, strictly speaking, is a zero-temperature phenomenon. A possible way to understand such a (de)-localization transition at finite temperature is to attribute the change in disorder due to variation in temperature; however a clear connection between the two is not very apparent. In QCD, varying the temperature also results in the sequential (effective) restoration of different subgroups of chiral symmetry. Evidence suggests that the restoration of the $SU_A(2)$ occurs through a second-order phase transition in the chiral limit [18]. The effective restoration of $U_A(1)$ will result in characteristic changes in the localization properties of the Dirac eigenvectors, on the other hand an Anderson-like transition also results in structural changes in the eigenvectors of the Dirac operator [74]. It is thus imperative to disentangle these two phenomena and to unambiguously identify the mechanism that drives these effects. However, the temperature regimes where these occur overlap with each other which makes it challenging to unambiguously separate these two effects.

In this chapter, we revisit the study of the eigenspectrum of the QCD Dirac operator on the lattice, but with fermion discretizations which have nearly exact chiral symmetry even on a finite lattice. We will examine how robust our conclusions about the fate of $U_A(1)$ discussed in Chapter 2. Additionally, we provide a new way of disentangling the impact of *effective* restoration of $U_A(1)$ and the gradual onset of localization in the 1-particle quark states as a function of temperature, through a detailed study of the Dirac eigenspectrum

on a lattice. We show here that though both these distinct physical phenomena affect the infrared part of the eigenspectrum of the QCD Dirac operator, at temperatures above T_{pc} , we discuss some discerning observables that can distinguish between the two. We demonstrate that the onset of localization at high temperatures due to disorder is distinct from the localization largely driven by topological fluctuations just above T_{pc} and can only be observed when the $U_A(1)$ subgroup of the chiral symmetry group is *effectively* restored.

We also measure for the first time the structural rigidity of the Dirac eigenstates calculated in terms of the curvature arising as a result of a twist applied to these eigenstates on one of the spatial boundaries of the lattice box [74]. It is well known that the curvature of eigenvalues of the Hamiltonian is related to the Thouless conductance [135]. We propose to use the analogue of the Thouless conductance for the Dirac eigenspectrum as a diagnostic tool for characterizing the *effective* restoration of anomalous $U_A(1)$ subgroup of the chiral symmetry in QCD.

4.2 Details of numerical lattice calculations

We calculate the eigenvalues and vectors of the massless overlap Dirac operator on gauge configurations of 2+1 flavor QCD generated using the Möbius domain wall discretization for fermions [44] and Iwasaki gauge action. This is because the overlap Dirac operator has an exact chiral symmetry on the lattice satisfies an index theorem and does not have additional lattice artifacts due to the breaking of chiral symmetry as in the case of Wilson fermions or the breaking of the continuum spin and flavor symmetries in staggered fermions. The computations were performed on a spacetime lattice which has $N_s = 32$ sites along each of the three spatial directions and $N_\tau = 8$ sites along the Euclidean temporal direction. The values of Möbius parameter c_5 at different temperatures were chosen such that the chiral symmetry violation for our chosen L_5 is minimal. The domain wall height

M_5 , was kept fixed at 1.8 for the entire set of simulations. The bare light and strange quark masses were chosen such that the pion mass is physical i.e., $M_\pi \sim 135$ MeV, and so is the kaon mass with $M_K \sim 495$ MeV [11]. The range of temperatures, $T = 1/(N_\tau a)$, we have studied is between 149-339 MeV, where a is the lattice spacing, such that the spatial extent $L = V^{1/3}$ is ~ 5.3 fm for $T = 149$ MeV whereas $L \sim 2.5$ fm for the highest temperature $T = 339$ MeV. Here the temperatures in physical units are expressed in terms of the Sommer parameter r_0 at each value of the gauge coupling g by relating it to the lattice spacing a through the two-loop beta-function [111].

The gauge configurations for $T \lesssim 181$ MeV were generated and used for calculating the disconnected piece of the chiral susceptibility and the pseudo-critical temperature $T_{pc} \simeq 158.7$ MeV [60]. However all gauge ensembles characterized by the bare parameter $\beta = 6/g^2$ for $\beta \gtrsim 1.829$ were generated from scratch. The temperature corresponding to $\beta = 1.829$ was already estimated in Ref. [111]. For precisely determining the temperature in MeV unit for the larger β values, we have first extracted the lattice spacing a in units of the mass of the omega baryon m_Ω [111, 136, 137] for a wide range of $\beta = 1.70$ -2.31. We next performed a fit of these extracted inverse spacings as a function of β and then use this fit and the 2-loop beta function to extract the corresponding temperatures in MeV for all β values. We checked that the temperature we extract out of this fit, corresponding to a lower $\beta = 1.633$, matches the value reported earlier [11]. Details of the parameters used in the configuration generation e.g., the Möbius parameter c_5 , the extent of the fifth dimension L_5 and the number of eigenvalues computed for each statistically independent configuration at different temperatures are mentioned in Table 4.1.

We use the massless overlap Dirac operator [40, 138] defined as $D_{ov} = 1 + \gamma_5 \text{sign}(\gamma_5 D_W(-M_5))$ where $D_W(-M_5)$ is the Wilson Dirac operator with the domain wall height $M_5 = 1.8$ appearing as a negative mass parameter. We have numerically implemented the overlap Dirac operator by representing the matrix sign function exactly in terms of the first 30 eigenvalues of $D_W^\dagger D_W$ and approximating it by a Zolotarev rational polynomial with 25

T (MeV)	β	c_5	L_5	N_s	N_τ	N_{eigen}	N_{confs}
149	1.671	1.5	16	32	8	100	40
159	1.707	1.5	16	32	8	100	44
164	1.725	1.5	16	32	8	100	95
177	1.771	1.0	16	32	8	100	93
186	1.801	1.0	16	32	8	90	57
195	1.829	0.9	16	32	8	100	108
270	2.130	0.5	24	32	8	150	122
314	2.250	0.5	12	32	8	200	111
339	2.310	0.5	12	32	8	200	92
SU(3)							
624	6.545	—	—	32	8	100	46

Table 4.1: Number of gauge configurations at different temperatures, $\beta = 6/g^2$ and lattice size used in this work. The table also lists the number of overlap Dirac eigenvalues calculated per gauge configuration, along with the values of the Möbius parameter c_5 and L_5 used in the generation of gauge ensembles at each temperature.

terms in the rest of the vector space. The numerical accuracy of our procedure ensures that the resultant overlap Dirac operator satisfies the Ginsparg-Wilson relation to a precision of $\lesssim 10^{-9}$ on each gauge configuration we have studied and the sign function is implemented to a numerical precision of 10^{-10} . As mentioned in Table 4.1, we typically calculate the first 90-200 non-zero eigenvalues of $D_{ov}D_{ov}^\dagger$, on each of the gauge configurations. The eigenvalues of the overlap Dirac operator are calculated numerically using the Kalkreuter-Simma Ritz algorithm with restarts. For optimization, we have first estimated the number and chirality of zero modes present per configuration and used this information to project the $D_{ov}D_{ov}^\dagger$ onto the opposite chirality sector. We then calculate the first 90-200 eigenvalues of this projected overlap Dirac operator and extract the eigenvalues of D_{ov} from them. We henceforth denote the imaginary part of the n -th eigenvalue as λ_n . We have also checked that the real part of the first $\mathcal{O}(200)$ overlap eigenvalues is about two orders of magnitude smaller and hence sub-dominant compared to their imaginary part. This allows us to directly relate our study to the continuum case where the Dirac operator has only imaginary eigenvalues.

We have also generated thermalized SU(3) gauge configurations (without dynamical quarks)

with the Wilson gauge action on $32^3 \times 8$ lattice and inverse coupling $\beta = 6/g^2 = 6.545$, which corresponds to a temperature $T \simeq 624$ MeV, about twice the deconfinement temperature $T_d \simeq 312$ MeV [139, 140]. The scale $r_0 = 0.4701(36)$ fm [133] is also used to set the temperature in this case. At this temperature the gluon degrees of freedom, especially below the magnetic scale are dominant, thus these gauge ensembles represent the physical scenario. The SU(3) gauge configurations at high temperatures were generated in order to compare how different a thermalized state is from a classical state of QCD which consists of highly occupied gauge fields [141, 142] with a non-thermal phase space distribution and without dynamical quarks.

4.3 Categorizing QCD Dirac eigenstates as *intermediate* and *bulk*

4.3.1 Level spacing ratios

We first calculate the spacings between neighboring eigenvalues of the overlap Dirac operator, denoted as $s_n = \lambda_{n+1} - \lambda_n$. Instead of calculating the level spacing distribution, we analyze the normalized ratios of consecutive level spacings, defined as $\tilde{r}_n = \min(r_n, 1/r_n)$, where $r_n = s_{n+1}/s_n$. The observable $\langle \tilde{r} \rangle$ is obtained at a given temperature, by averaging $\tilde{r}_n$ over all eigenvalues within a specific spectral window followed by an ensemble average over gauge configurations. Consequently, the index n is explicitly dropped after these averages are performed. This construction naturally eliminates the local dependence of the spacing distribution on the eigenvalue level density [143]. As a result, the ratio $\tilde{r}_n$ remains insensitive to the systematic errors that typically arise due to unfolding of the spacing distribution, particularly in small volumes or with limited statistics.

We now outline our procedure for categorizing the Dirac eigenvalues into different spectral windows. First, we calculate $\langle \tilde{r} \rangle$ in small bins of λ/T by averaging over the gauge

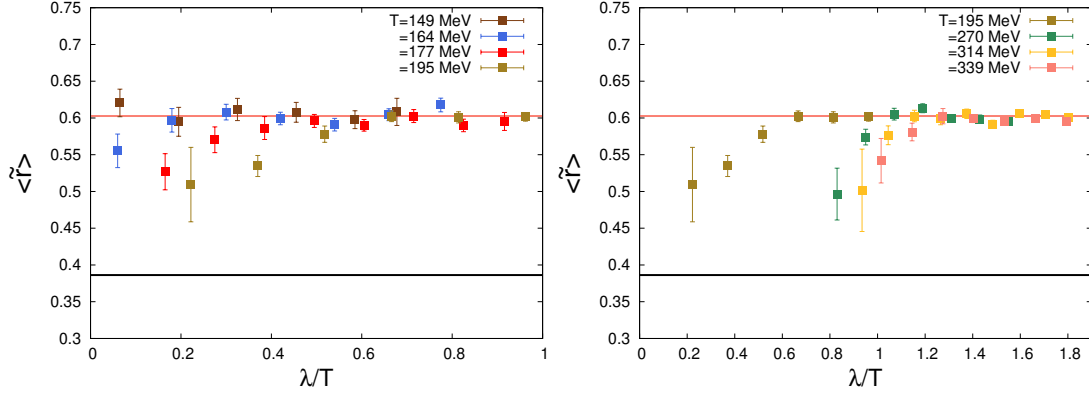


Figure 4.1: Left panel: The variation of $\langle \tilde{r} \rangle$ in bins of the Dirac eigenvalues λ/T in the temperature range close to the pseudo critical temperature where $U_A(1)$ part of the chiral symmetry is broken. Right panel: The variation of $\langle \tilde{r} \rangle$ in small bins in λ/T at high temperatures $T \gtrsim 270$ MeV when the $U_A(1)$ is *effectively* restored, compared to the data at 195 MeV. The orange and black solid lines in both panels represent the expected $\langle \tilde{r} \rangle$ for the eigenvalues with GUE and Poisson level statistics respectively.

configurations at each temperature. The results for $\langle \tilde{r} \rangle$ in bins of λ/T close to and much above the chiral crossover transition are summarized in Fig. 4.1. Note that the upper cutoff for these spectral windows is determined by the maximum eigenvalue calculated at a given temperature. Focusing on $T = 164$ MeV which lies just above T_{pc} , we observe that the value of $\langle \tilde{r} \rangle$ in the lowest bin lies between the expectations from an uncorrelated ensemble and a GUE; we classify them as *intermediate* eigenmodes. Conversely, bins where $\langle \tilde{r} \rangle = 0.60266$ within errors are classified as *bulk* eigenmodes. This categorization can be straightforwardly extended to all other temperatures. Specifically, at temperatures $T = 154, 164, 177, 186$, and 195 MeV, all eigenmodes below $\lambda/T = 0.08, 0.12, 0.33, 0.5$, and 0.6 , respectively, are designated as *intermediate* eigenmodes, while those above these thresholds are identified as *bulk* eigenmodes. For $T < T_{pc}$ the values of $\langle \tilde{r} \rangle$ in the deep infrared part of the spectrum can be explained within the universality class of RMT consisting of chiral Gaussian unitary ensemble (GUE) [55–58] whereas for the higher eigenvalue bins the universal features can be explained within Wigner’s classification with a RMT ensemble of conventional GUE.

At even higher temperatures $T > T_{U(1)}$ —where $T_{U(1)} \sim 1.5T_{pc}$ marks the temperature above which the $U_A(1)$ part of the chiral symmetry is effectively restored [59]—we expect

Dirac eigenvalues arising from a dilute instanton gas gauge background to accumulate in the deep infrared region of the spectrum [61, 81], separating from the bulk via a spectral gap. We observe this gap opening as the temperature increases beyond 195 MeV in the right panel of Fig. fig:rtildavslambda. Notably, the values of $\langle \tilde{r} \rangle$ in the lowest bins, starting around $\lambda/T = 0.5, 0.6$, and 0.85 for temperatures $T = 270, 314$, and 339 MeV, respectively, exhibit large statistical noise due to the rare occurrence of such eigenvalues. Therefore, they are excluded from our plot of normalized level ratios in the right panel of Fig. 4.1. Consequently, we characterize all eigenmodes with $\lambda/T < 1.0, 1.1$, and 1.2 at $T = 270, 314$, and 339 MeV, respectively, as *intermediate* eigenmodes, since their $\langle \tilde{r} \rangle$ values fall between those of a GUE and an uncorrelated matrix ensemble. Eigenvalues exceeding these thresholds constitute the bulk eigenspectrum.

For clarity, we now go beyond the bin-by-bin analysis of $\langle \tilde{r} \rangle$ shown in Fig. 4.1. Instead, in the left panel of Fig. 4.2 we show the resulting $\langle \tilde{r} \rangle$ for the entire window of *intermediate* and *bulk* eigenmodes as a function of temperature, represented by blue and red points, respectively. The eigenvalues in the lowest bins for $T > T_{pc}$ exhibit distinct characteristics that separate them from the bulk eigenspectrum, which maintains an average value of $\langle \tilde{r} \rangle \approx 0.602$, consistent with GUE expectations [144]. Thus the bulk eigenmodes characterize the chaotic part of the QCD Dirac eigenspectrum. The emergence of these *intermediate* eigenmodes just above T_{pc} has important physical consequences, which will be discussed in a later Section 4.6 of this chapter. At these temperatures, the singlet $U_A(1)$ subgroup remains significantly broken [60], leaving only a remnant Z_2 subgroup of the chiral symmetry intact.

To verify that the bulk eigenmodes have been correctly identified thus the robustness of our categorization procedure, we also calculate the probability distribution of nearest-neighbor spacing ratios [144, 145]. This quantity, like $\langle \tilde{r} \rangle$, is independent of the unfolding procedure and can be directly compared to the GUE prediction, $P(r) = \frac{11.16 (r+r^2)^2}{(1+r+r^2)^4}$. As shown in the right panel of Fig. 4.2, the bulk eigenmodes defined by our criterion strictly

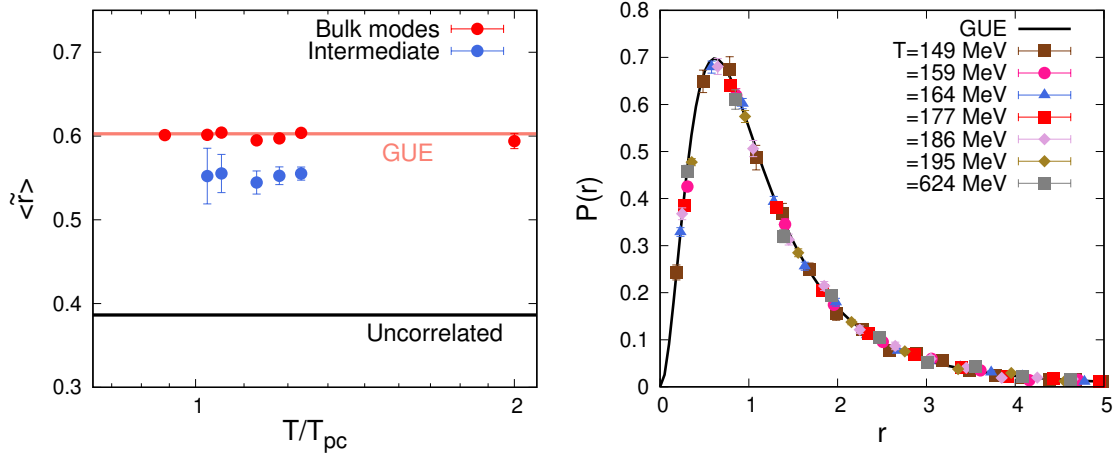


Figure 4.2: Left panel: Average value $\langle \tilde{r} \rangle$ in different spectral windows defined in terms of the overlap Dirac eigenvalues at various temperatures T . Red and blue points correspond to bulk and *intermediate* eigenmodes, respectively. The results are compared with the theoretical expectations for the GUE and completely uncorrelated (Poisson) spectra, shown as red and black horizontal lines, respectively. Right panel: Probability distribution of ratios of consecutive level spacings for bulk eigenmodes at different temperatures with and without dynamical quarks. Note that for pure SU(3) gauge ensemble at $T = 624$ MeV, the T_{pc} represents the deconfinement temperature T_d .

follow the GUE prediction across all temperatures.

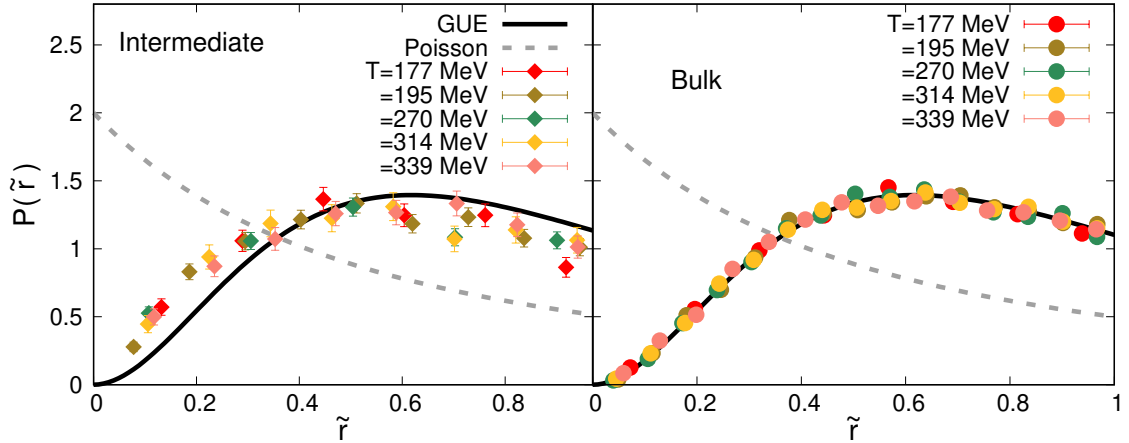


Figure 4.3: Probability distribution of $\tilde{r}$ for the *intermediate* (left) and bulk (right) eigenvalues at different temperatures compared with its values for random matrices belonging to GUE (solid line) and those belonging to uncorrelated eigenvalues following Poissonian level statistics (dotted line).

We next investigate the probability distribution of normalized level ratios, $P(\tilde{r})$. Since $\tilde{r}$ is bounded between 0 and 1, we can include all data points unlike $P(r)$ shown earlier in Fig. 4.2. Our lattice results for $P(\tilde{r})$ for eigenvalues in the infrared part of the QCD

Dirac spectrum, compiled in Fig. 4.3, offer key insights into their localization properties across different temperatures. The left panel displays the probability distribution for the *intermediate* region of the Dirac spectrum, while the right panel shows the probability distribution for the bulk region. As expected, $P(\tilde{r})$ for bulk eigenmodes at all temperatures perfectly matches predictions from the GUE. However, $P(\tilde{r})$ for *intermediate* eigenvalues differs significantly from both uncorrelated eigenvalues and the GUE.

These observations pose two main questions: What is the physical origin of these *intermediate* eigenvalues, and can their properties be explained using a matrix model like the bulk eigenvalues? We address these questions in a later Section 4.5 of this chapter. As we already observed in our study of the HISQ Dirac eigenspectrum [69], the degree of this mixing depends on the temperature. In fact, these *intermediate* eigenmodes proliferate when $SU_A(2)$ symmetry is effectively restored as discussed in Chapter 2.

4.3.2 Localization properties

We next study the localization properties of the Dirac eigenstates, which for a particular eigenstate $\psi(\mathbf{x})$ is quantified in terms of the generalized Rényi entropy defined as,

$$R_\alpha = \frac{1}{1-\alpha} \ln \sum_{\mathbf{x}} p_{\mathbf{x}}^\alpha, \quad 1 \leq \alpha < \infty. \quad (4.1)$$

The quantity $p_{\mathbf{x}} = |\psi(\mathbf{x})|^2$ denotes the probability density of an eigenstate at a spatial position $\mathbf{x}$ obtained after averaging the four-dimensional density over τ . Our lattice results for the first Rényi entropy R_1 normalized by the logarithm of the spatial volume, for each eigenvalue bin, are compiled in the top panel of Fig. 4.4. It is evident that the bulk eigenmodes have significantly higher values ranging between $0.92 < R_1/\log V < 1.0$, approaching unity at the highest temperature i.e., 624 MeV. This implies that the bulk eigenmodes are almost completely delocalized over the spatial volume and thus are ergodic, containing equivalent thermal information in each of them. This is an indirect

manifestation [146] of the ETH, which has been demonstrated in non-Abelian theories in 2+1 dimensions [147, 148]. Whereas for temperatures $T = 159\text{--}195$ MeV, the *intermediate* eigenmodes do not contain the entire thermodynamic information that is encoded in the bulk eigenmodes, as evident from their values of $R_1/\log V$. These *intermediate* eigenmodes are thus not as delocalized as bulk eigenmodes, hence not fully ergodic.

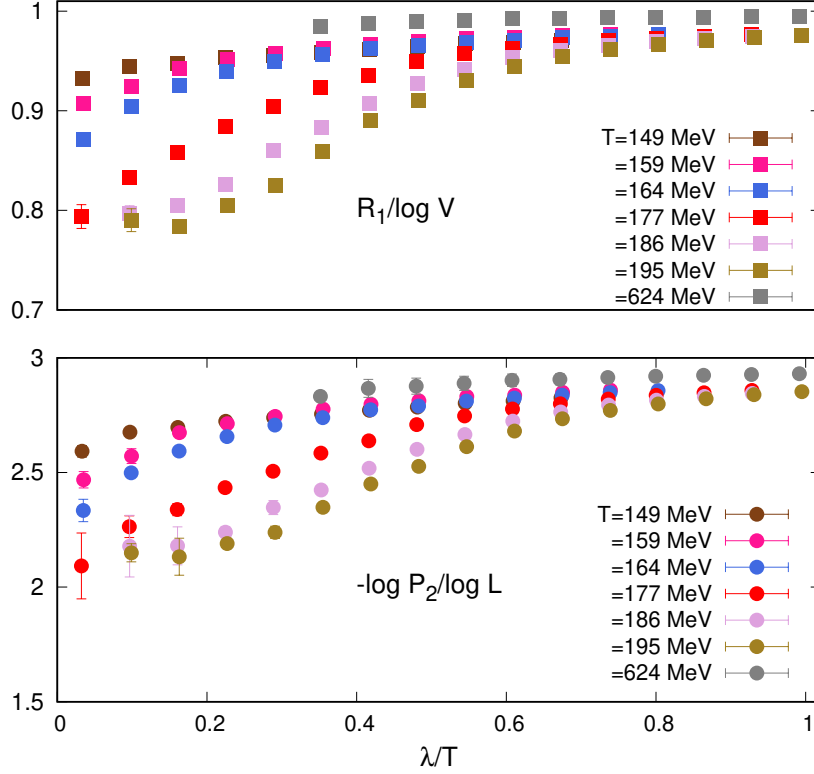


Figure 4.4: Variation of first Rényi entropy (top panel) and D_2 (bottom panel), for eigenvectors binned in λ/T for different temperatures, performed on the gauge configurations mentioned in Table 4.1.

To further understand the localization properties of the *intermediate* eigenmodes, we study the inverse participation ratio (IPR) defined as $P_2 = \sum_{\mathbf{x}} |\psi(\mathbf{x})|^4$. For a completely delocalized eigenstate we expect its P_2 to ideally scale as the inverse of the volume of the system as L^{-3} which might be spoiled by the presence of thermal fluctuations. The results for $D_2 = -\log P_2/\log L$ as a function of bins in λ/T are shown in the lower panel of Fig. 4.4 which demonstrates different volume scaling for the bulk and *intermediate* eigenmodes.

Apart from the local correlations that are observed e.g., in the spacing ratios, it is also important to identify any global correlations that exist among eigenvalues. Such correlations will give rise to distinct structural properties of different regimes of the Dirac eigenspectrum as a function of temperature and it is important to understand their physical origin. One such quantity which can quantify the global correlation is the curvature K which is defined in terms of the change in the properties of the Dirac eigenstates ψ_i subject to a twist η along any of the spatial directions, denoted as $\psi_i(x + L) = \psi_i(x)e^{i\eta}$. As a result, each eigenvalue labeled by an index i will acquire a curvature K_i defined as,

$$K_i = \lim_{\eta \rightarrow 0} \left| \frac{\partial^2 \lambda_i}{\partial \eta^2} \right|. \quad (4.2)$$

We calculate the probability distribution of curvature values $P(K)$ of the *intermediate* and bulk eigenmodes separately by subjecting these to a small twist $\eta = 0.005$. This is performed by choosing appropriate bins in terms of the normalized curvature values $K_i \rightarrow K_i/\langle K \rangle$ for *intermediate* and bulk eigenmodes, respectively. After performing an ensemble average over the gauge configurations, the results obtained for $P(K)$ are shown as a function of K for four different temperatures in Fig. 4.5. Bulk eigenstates which are delocalized over the entire volume are expected to acquire larger curvature upon applying a twist. In comparison *intermediate* eigenstates which are delocalized but not ergodic should mildly depend on the twist applied at the boundaries of the lattice box, if at all, will acquire a small curvature. There can, however, be rare fluctuations in the curvature distribution due to localized eigenstates that might be situated close to the boundaries of the lattice box. Our lattice data for the curvature distribution of the *intermediate* and bulk eigenmodes, shown in the left and right panels respectively of Fig. 4.5, are consistent with these expectations. In order to quantify how close bulk eigenstates are to the GUE predictions, we compare their curvature distribution with that of the eigenstates of random matrices belonging to GUE [149], given as $P(K) = \frac{2}{\pi} \frac{1}{(K^2+1)^2}$. As evident from Fig. 4.5, there is a fairly good agreement between $P(K)$ for bulk eigenmodes with the prediction

from a GUE, at different temperatures. We have also verified that the curvature distribution at a different twist $\eta = 0.01$ is consistent with the results obtained with $\eta = 0.005$, confirming that our conclusions are free from systematic uncertainties arising due to not-so-small choice of the twist parameter.

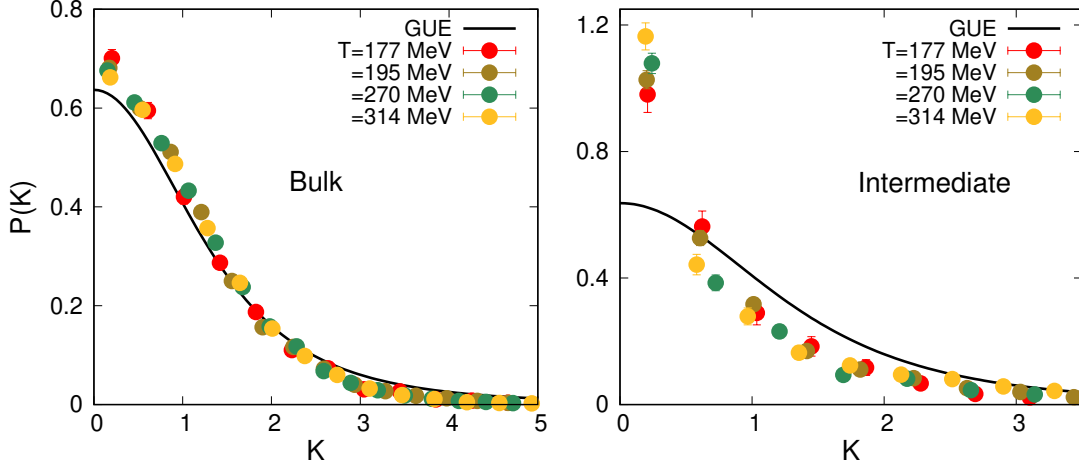


Figure 4.5: The curvature distribution of the bulk (left) and *intermediate* Dirac eigenmodes (right) as a function of temperature. The black solid line represents the expected probability distribution for the curvature K for eigenvalues of random matrices belonging to a GUE.

4.4 A matrix model interpretation of the *intermediate* Dirac eigenmodes

As anticipated in the Section 4.3, one of the simplest ways to explain the observed $P(\tilde{r})$ for *intermediate* eigenmodes shown in Fig. 4.3 could be in terms of an admixture of uncorrelated eigenvalues with the eigenvalues of matrices belonging to the GUE. In this section we discuss the construction of a matrix model that can quantitatively account for the $P(\tilde{r})$ for *intermediate* Dirac eigenmodes.

We follow three different approaches to model the distribution of $\tilde{r}$ for the *intermediate* eigenvalues in the same spirit as but by extending concepts from the random matrix theory. We construct our models starting with a random matrix belonging to GUE with 0.3

million eigenvalues. The probability distribution $P(\tilde{r})$ for the level ratios should follow the GUE prediction, which is confirmed and shown in Fig. 4.6 as a black solid line. As our first model, we construct a sufficiently small block of eigenvalues drawn from a uniform random distribution with a spacing distribution akin to uncorrelated eigenvalues following Poisson statistics whose size is 3% and 15% of the GUE block respectively. The eigenvalues of this block are chosen such that they lie within the range of the eigenvalues present in the GUE block except at the edges of this range, in order to allow for a complete mixture of the uncorrelated and GUE eigenvalues without any leakage. This is also done to mimic the QCD Dirac spectrum as closely as possible, where we do not observe any localized uncorrelated eigenvalues. Whenever a new eigenvalue is inserted in between existing eigenvalues of the GUE block, three new normalized level ratios arise as a result denoted as $\tilde{r}_{n_1}, \tilde{r}_{n_2}, \tilde{r}_{n_3}$. In order to be more explicit, let us assume that a new eigenvalue $\lambda_{n'}$ is inserted between the existing eigenvalues λ_n and λ_{n+1} of the GUE block such that the spectrum of the new mixed ensemble is denoted by $\lambda_0, \lambda_1, \dots, \lambda_{n-1}, \lambda_n, \lambda_{n'}, \lambda_{n+1}, \lambda_{n+2}, \dots, \lambda_{N-1}$. Here λ_i , where $i = 0, \dots, N-1$ are eigenvalues of our original GUE-block of size N . The three new level ratios that arise as a result are $r_{n_1} = \frac{\lambda_{n'} - \lambda_n}{\lambda_n - \lambda_{n-1}}$, $r_{n_2} = \frac{\lambda_{n+1} - \lambda_{n'}}{\lambda_{n'} - \lambda_n}$ and $r_{n_3} = \frac{\lambda_{n+2} - \lambda_{n+1}}{\lambda_{n+1} - \lambda_{n'}}$, which are normalized to give us $\tilde{r}_{n_i} = \min\left(r_{n_i}, \frac{1}{r_{n_i}}\right)$, $i = 1, 2, 3$. The new eigenvalues are accepted only if all three locally induced $\tilde{r}$ are compatible with the target distribution i.e. $P_{\text{GUE}}(\tilde{r})$, implemented through an independent accept-reject criterion. The acceptance probability of this newly selected eigenvalue is set to be $\prod_{i=1}^3 \frac{P_{\text{GUE}}(\tilde{r}_{n_i})}{P_{\text{GUE}}^{\max}}$, where $P_{\text{GUE}}(\tilde{r})$ is the probability distribution of normalized ratios $\tilde{r}$ for matrices belonging to GUE whereas $P_{\text{GUE}}^{\max}$ is the maximum value possible for the distribution $P_{\text{GUE}}(\tilde{r})$.

Although the probability with which each new eigenvalue is accepted is same as that of a GUE, for a sufficiently small block size of these newly chosen eigenvalues it is obvious that the level repulsion between them is consistent with a Poisson distribution, as apriori no correlations exist between them. The probability distribution $P(\tilde{r})$ for the eigenvalues within this new block with block sizes 3% and 15% of the GUE-block respectively are also shown in Fig. 4.6. From the plot it is clearly evident that for a smaller block which

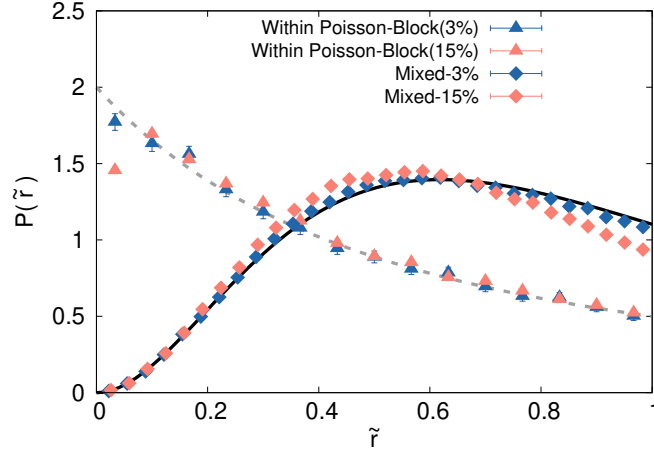


Figure 4.6: The probability distribution of the normalized level ratios $P(\tilde{r})$ for our first matrix model where a GUE block is additionally mixed with a block of uncorrelated eigenvalues following level statistics similar to a Poisson distribution selected with a probability distribution weight for $\tilde{r}$ determined according to random matrices belonging to a GUE. The $P(\tilde{r})$ for the newly added uncorrelated block, and the entire mixed matrix are shown as triangles and diamonds respectively denoting 3% (blue) and 15% (orange) admixture. The $P(\tilde{r})$ for eigenvalues belonging to uncorrelated and GUE matrices are shown as dashed and solid lines respectively.

is 3% of the original GUE-block, the $P(\tilde{r})$ agrees well with that known for a Poisson distribution. In the same figure, we have also shown $P(\tilde{r})$ for the full spectrum where existing eigenvalues from a GUE-block has an admixture of 3% and 15% of its size from the uncorrelated block, labeled as *mixed*. From Fig. 4.6 it is evident that this model cannot explain the $P(\tilde{r})$ for the *intermediate* Dirac eigenmodes shown in Fig. 4.3 for smaller values of $\tilde{r}$.

Our second model is designed in a similar manner as the first one but in this case the randomly chosen new eigenvalues are accepted within the existing GUE-block with a probability $\prod_{i=1}^3 \frac{P_P(\tilde{r}_{n_i})}{P_P^{\max}}$. Here $P_P(\tilde{r})$ is the probability distribution of normalized level ratios $\tilde{r}$ for uncorrelated eigenvalues following Poisson level statistics whereas $P_P^{\max}$ is the maximum possible value for the distribution $P_P(\tilde{r})$. In this approach, eigenvalues that are closely spaced will be more favored. We show the results of our calculation of $P(\tilde{r})$ in Fig. 4.7, when the newly added eigenvalue block are of sizes which are 3% and 15% respectively of the original GUE block. The $P(\tilde{r})$ of the newly added eigenvalue block

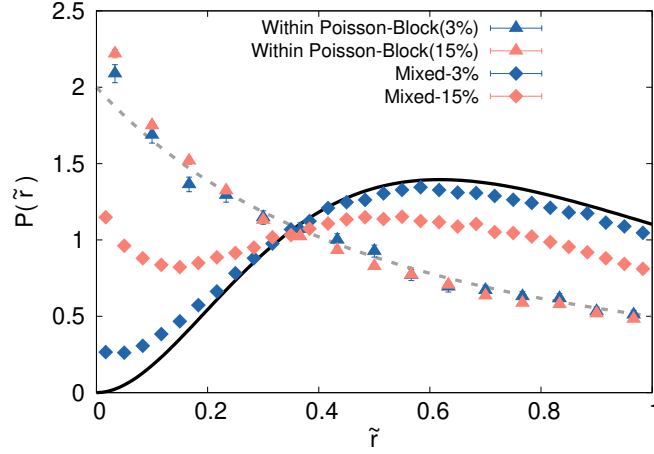


Figure 4.7: The $P(\tilde{r})$ for our second matrix model where a GUE block is additionally mixed with a block of uncorrelated eigenvalues selected with a probability distribution weight for $\tilde{r}$ determined from a Poisson distribution. The $P(\tilde{r})$ for the newly added uncorrelated block, and the entire *mixed* matrix are shown as triangles and diamonds respectively denoting 3% (blue) and 15% (orange) admixture. The $P(\tilde{r})$ for eigenvalues belonging to uncorrelated and GUE matrices are shown as dashed and solid lines respectively.

is close to the value for uncorrelated eigenvalues, as expected. The $P(\tilde{r})$ of the entire matrix consisting of GUE and Poisson blocks are labeled as *mixed* and is also shown in same figure. For smaller values of $\tilde{r}$, the $P(\tilde{r})$ is intermediate between the values expected from Poisson and GUE level statistics respectively, which is quite different from the trend observed for *intermediate* eigenvalues of the QCD Dirac spectrum at all temperatures. This motivates us to formulate a third approach.

Our third approach will focus on improving the modeling of $P(\tilde{r})$ to more closely mimic the lattice data at smaller values of $\tilde{r}$. Our lattice data for *intermediate* eigenvalues shows some enhancement of $P(\tilde{r})$ compared to its magnitude in GUE for moderately small values of $\tilde{r}$ but the probabilities for the existence of eigenvalues with negligibly small spacing ratio $\tilde{r} \rightarrow 0$ are heavily disfavored. We model this fact in our random matrix construction by accepting newly generated eigenvalues with a probability $\prod_{i=1}^3 P_{\text{mix}}(\tilde{r}_{n_i})$, where $P_{\text{mix}}(\tilde{r}) \in \left\{ \frac{P_{\text{GUE}}(\tilde{r})}{P_{\text{GUE}}^{\text{max}}}, \frac{P_{\text{P}}(\tilde{r})}{P_{\text{P}}^{\text{max}}} \right\}$. Which of the two elements in this set decides the probability of accepting an eigenvalue depends on the values of $\tilde{r}_{n_1}, \tilde{r}_{n_2}, \tilde{r}_{n_3}$ and a threshold value of $\tilde{r}_{\text{max}}$ chosen in our study to be $\tilde{r}_{\text{max}} = 0.05$. If values of $\tilde{r}_{n_1}, \tilde{r}_{n_2}, \tilde{r}_{n_3} < 0.05$ then the

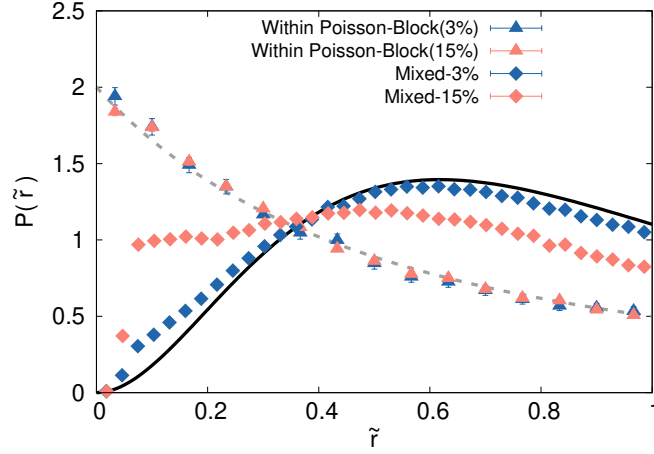


Figure 4.8: The $P(\tilde{r})$ for our third matrix model where a GUE block is additionally mixed with a block of uncorrelated eigenvalues selected with a probability distribution weight for $\tilde{r}$ for a mixed distribution (see text for details). The $P(\tilde{r})$ for the newly added uncorrelated block, and the entire mixed matrix are shown as triangles and diamonds respectively denoting 3% (blue) and 15% (orange) admixture. The $P(\tilde{r})$ for eigenvalues belonging to uncorrelated and GUE matrices are shown as dashed and solid lines respectively.

$P_{\text{mix}}(\tilde{r}_{n_i}) = P_{\text{GUE}}(\tilde{r}_{n_i})$ else $P_{\text{mix}}(\tilde{r}_{n_i}) = P_P(\tilde{r}_{n_i})$. This selection criterion thus explicitly avoids selecting new eigenvalues which will lead to proliferation of smaller values of $\tilde{r}$. The probability distributions $P(\tilde{r})$ for the newly added eigenvalues constituting a block of size 3% and 15% of the existing GUE block respectively for this *mixed* model are shown in Fig. 4.8. For the smaller block size of the newly accepted eigenvalues which comprises 3% of the original GUE-block, the repulsion among the closely spaced eigenvalues is similar to expectations in a Poisson ensemble. In the same figure, we have also compiled our results for $P(\tilde{r})$ of the entire matrix consisting of both GUE and uncorrelated blocks which we consistently label as *mixed*. The $P(\tilde{r})$ for the eigenvalues chosen in this hybrid approach with an 3-15% admixture can explain our lattice data for the normalized level ratios of *intermediate* Dirac eigenvalues for a wide range of temperatures between 177-339 MeV. This is shown in Fig. 4.9 where the band represents the prediction from our model 3 with an admixture in the range $\sim 3\text{-}15\%$. Note however that the amount of admixture might vary within each small bins in λ/T and its precise determination in the far infrared part of the spectrum will require further improvement in statistics.

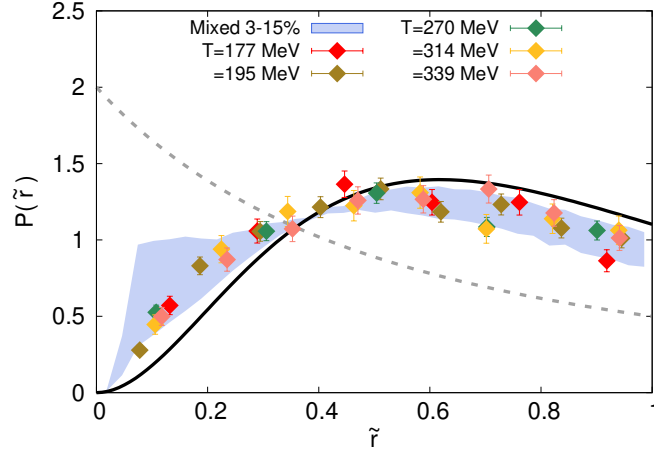


Figure 4.9: The probability distribution of $\tilde{r}$ at different temperatures for *intermediate* Dirac eigenmodes compared to the values obtained in our matrix model 3 shown as a blue band. The band represents values of $P(\tilde{r})$ corresponding to 3-15% mixing described within our matrix model 3. The $P(\tilde{r})$ for eigenvalues belonging to uncorrelated and GUE matrices are shown as dashed and solid lines respectively.

We will now elaborate on a physical understanding of these models, i.e. why our model 3 can realistically describe the universal level spacing ratios for the *intermediate* Dirac eigenvalues in different temperature regimes. Dyson provided an intuitive understanding [150] of the level spacing distribution of eigenvalues ϵ_i of a $N \times N$ random matrix by modeling them as fictitious Brownian point particles moving in one dimension at finite temperature, whose inverse is the Dyson index β . The potential that describes the Brownian motion of the eigenvalues consists of a confining as well as a repulsive part given by $V(\{\epsilon_i\}) = \sum_{i=1}^N \epsilon_i^2 - \sum_{i < j} \log |\epsilon_i - \epsilon_j|$, where i, j label the eigenvalues. Performing a Monte-Carlo simulation of this system consisting of $N = 1000$ Brownian particles, the distribution of the normalized level spacing ratios of a random matrix belonging to GUE can be reproduced for $\beta = 2$.

Now, in order to understand the origin of *intermediate* level statistics in terms of Dyson's construction, we replace the harmonic oscillator potential with another choice which causes a weaker confinement [151, 152]. The choice of different weak confining potentials was originally motivated in order to construct different classes of random matrix ensembles that have multi-fractal eigenfunctions and to understand what characteristic

signatures of such multifractality are inherent in the spacing distribution [152]. For one such choice of a confining potential, $V(\{\epsilon_i\}) = A \sum_i \ln^2 |\epsilon_i|$, we obtain a normalized level spacing ratio distribution which can very well explain our lattice data for the *intermediate* Dirac eigenvalues, shown in Fig. 4.10. We have verified that level spacing ratio distributions are independent of the strength of potential denoted by A , by varying it sufficiently $A \in [0, 10]$. However the results discussed here are for $A = 0.2$. Another different choice of a weaker confining potential [151], $V(\{\epsilon_i\}) = A \sum_i |\epsilon_i|^\alpha$ can explain our lattice data consistently as well.

Similar analysis for the distribution of level ratios have been performed on a mixed ensemble of Poisson-GOE matrices in Ref. [153] by generalizing the techniques formulated in Ref. [154] for understanding mixing between eigenvalues of matrices belonging to different symmetry classes [155]. These works [153, 154] derive the joint distribution of consecutive nearest-neighbor level spacings of a compound spectrum constructed out of spectra with different distributions. However for a Poisson-GUE system there is no analytic solution available for the normalized level spacing ratios in this approach, which have to be determined numerically. Our numerical approach is thus a different way to explain a mixed ensemble of matrices of two symmetry categories. We also note that modeling a mixed level-spacing distribution has also been discussed in the literature heuristically in terms of a best fit function with few parameters [156]. A microscopic model consisting of a two-dimensional matrix mimicking a Poisson process weakly coupled with a random matrix belonging to different Wigner surmise [157–159] has also been shown to fit a mixed distribution in terms of a single parameter that denotes the strength of the coupling.

We conclude this section by summarizing our procedure to understand the onset of the *intermediate* region observed in the QCD Dirac eigenspectrum starting from predominantly chaotic eigenvalues in the bulk. By varying the fractional admixture of uncorrelated eigenvalues introduced within a large GUE matrix block according to a very specific criterion which is discussed above in model 3, one can very well describe the values of $\langle \tilde{r} \rangle$

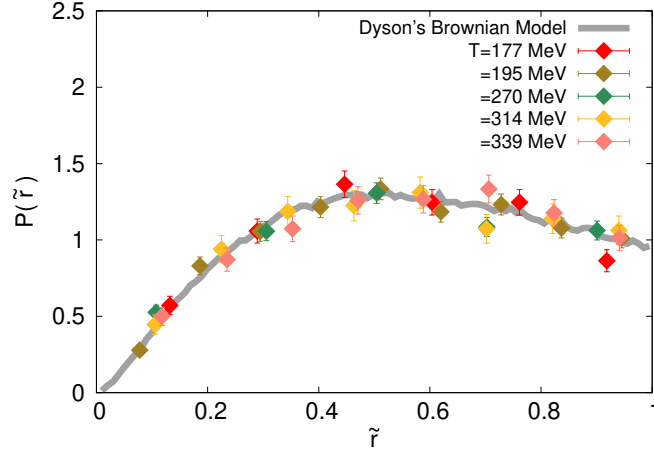


Figure 4.10: The probability distribution for $\tilde{r}$ obtained using Dyson's Brownian model for eigenvalues $\{\epsilon_i\}$ moving in presence of a weak confining potential along with a log-repulsion between them shown as a solid line. The probability distributions of $\tilde{r}$ for the Dirac eigenvalues with *intermediate* level statistics, at different temperatures are also shown (as points) for comparison.

for the *intermediate* eigenmodes. The matrix model in turn has a nice interpretation in terms of Dyson's construction of a Brownian model of eigenvalues. Our construction is very general and versatile, which can describe the probability distribution $P(\tilde{r})$ for *intermediate* eigenvalues appearing as a result of different physical mechanisms at work at different temperatures. Compared to $T = 195$ MeV one observes that the values of $\langle \tilde{r} \rangle$ at $T = 314$ MeV deviates from the bulk more dramatically within a span of few bins while moving towards the infrared. Typically at temperatures $T < T_{U(1)}$ when the (anomalous) singlet subgroup of chiral symmetry is not *effectively* restored, the contribution of uncorrelated eigenvalues varies slowly as a function of λ , gradually increasing in the most infrared bins. At $T \simeq T_{U(1)}$ the *intermediate* values of $\langle \tilde{r} \rangle$ are visible only in the lowest few eigenvalue bins and those tend to be even more closer to an uncorrelated distribution.

4.5 Origin of (de)localization of the Dirac eigenstates

Having interpreted the Dirac eigenmodes with *intermediate* level statistics as arising due to an admixture between eigenvalues with universal level spacing fluctuations of GUE and

Poisson type, we would now like to understand the microscopic origin of such a mixing.

We recall that in the Euclidean formalism the partition function of QCD can be realized as a path integral with fermion fields satisfying anti-periodic boundary conditions along the compact imaginary time of extent $1/T$. As a result the lowest eigenvalue of the Euclidean lattice Dirac operator for non-interacting quarks is $\sin(\pi/N_\tau)$. Turning on gauge interactions, the temporal part of the Dirac operator can be diagonalized in the limit of weak coupling, the diagonal elements at each lattice site depends on the lowest Matsubara mode shifted by the local Polyakov loop values [159]. A random matrix model of these local Matsubara modes with nearest-neighbor interactions closely resembles the tight-binding Anderson model [159]. At high temperatures the fluctuations of the Polyakov loop around its mean become rarer and occur at random spatial locations [63, 107, 160], justifying its resemblance with a random disorder. The randomness in the gauge field background is solely driven by the inherent chaotic nature of classical color fluctuations at these temperatures [161, 162]. However the validity of these assumptions needs to be revisited for temperatures $T_{pc} < T < T_{U(1)}$.

Since the gauge field configurations represent a strongly interacting many-body system at $T_{pc} < T < T_{U(1)}$ it is not clear apriori whether the noise inherent in it can be considered as random, as required in an Anderson model. In this regime regions of strong fluctuations in the local values of the Polyakov loop which have been demonstrated to be anti-correlated with the probability density for the occurrence of instanton-dyons [163] which form a semi-classical gas [164, 165]. Hence the origin of disorder at temperatures T_{pc} is largely driven by fluctuations about the topological vacuum in QCD and is very different from a random uncorrelated distribution since the temperature dependence of the topological susceptibility is distinct from a dilute instanton gas [59].

The generalization of Anderson localization in interacting systems, known as many-body localization [100] has been discussed as a finite temperature phase transition and is currently under intensive review [166, 167]. The characteristic signatures of a (de)-

localization transition in such interacting systems have been shown to be manifest in different single particle observables as well [93]. Furthermore, the disorder inherent in the gauge fields in QCD is a function of temperature, as these are not quenched (static) but dynamically generated due to self interactions similar to a scenario discussed in the context of interacting lattice spins models [168].

We would also like to remind here that when we calculate eigenvectors of the Dirac operator in the presence of a noisy gauge background, we are solving for relativistic single particle states. This is different from a conventional Anderson model which discusses non-relativistic electrons in the presence of a quenched random potential. The Anderson transition has been studied in three-dimensional non-interacting Dirac semimetals in the presence of quenched disorder [169]. It was reported that such systems have three distinct ground states, i.e., an incompressible semimetal, a compressible diffusive metal, and an insulator, which is in contrast to a conventional Anderson model that describes a transition between only the latter two phases. In the presence of a small amount of disorder, there is a quantum phase transition from a semimetal to a dirty metal phase which, on increasing disorder strength by about six times, goes over to an insulating phase through the conventional Anderson semimetal-insulator transition. In quenched SU(3) gauge theory at $T \sim 600$ MeV, we do not observe any localized Dirac eigenstates in the deep infrared part of the spectrum [73], which might be due to the weakening of the disorder in the gauge fields. Hence it is imperative that we make a more quantitative estimate of the amount of disorder inherent in the gauge fields, as a function of temperature in the context of QCD.

We will now investigate if the origin of *intermediate* eigenvalues in the temperature regime $T > T_{U(1)}$ is intimately correlated with the disorder inherent in the gauge fields, which is typically quantified in terms of fluctuations around the average renormalized Polyakov loop values [107] at each spatial position. We also study how the typical magnitude of these fluctuations vary as a function of temperature, especially in the temperature regime $T_{pc} < T < T_{U(1)}$.

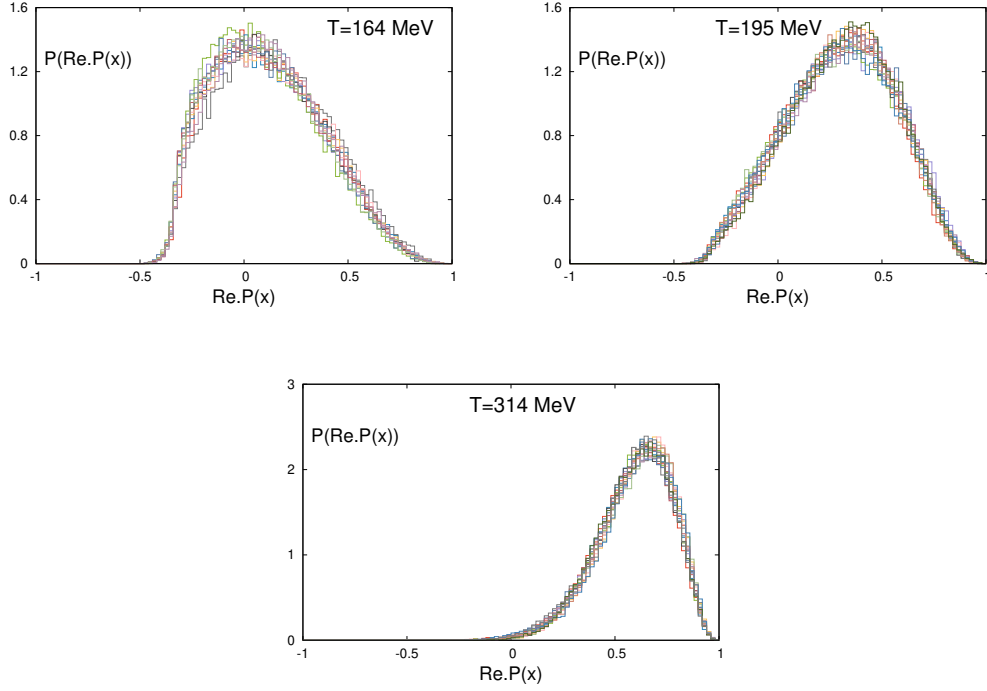


Figure 4.11: Probability distribution of the $\text{Re}.P(\mathbf{x})$ for statistically independent gauge configurations, calculated after performing Wilson flow renormalization at three different temperatures above the chiral crossover transition.

For this purpose, we have calculated the renormalized Polyakov loop values at each spatial site for different temperatures, after performing gradient flow using the Wilson gauge action [170]. The flow equation is solved using the fourth-order Runge-Kutta scheme with a step size of 0.01 up to a flow time t which should ideally be determined from the criterion $a \ll \sqrt{8t} \ll 1/T$. To ensure that this criterion is satisfied for all temperatures we have studied, the flow time in physical units was chosen to be $\sqrt{8t} = 0.44$ fm for $T \leq 195$ MeV and $\sqrt{8t} = 0.25$ fm for higher temperatures $T > 200$ MeV. We applied a constant shift in free energy to match with the earlier continuum extrapolated results from Ref. [171] at the highest temperature in order to fix the scale. This same shift in the free energy values for two lower temperatures 270 and 314 MeV also gave us an estimate of the renormalized Polyakov loop, which is in good agreement with the continuum results mentioned in Ref. [171].

We show the probability distribution of renormalized values of the real part of the Polyakov loop at each site $\mathbf{x}$ denoted as of $\text{Re}.P(\mathbf{x})$ for a large set of gauge configurations and at

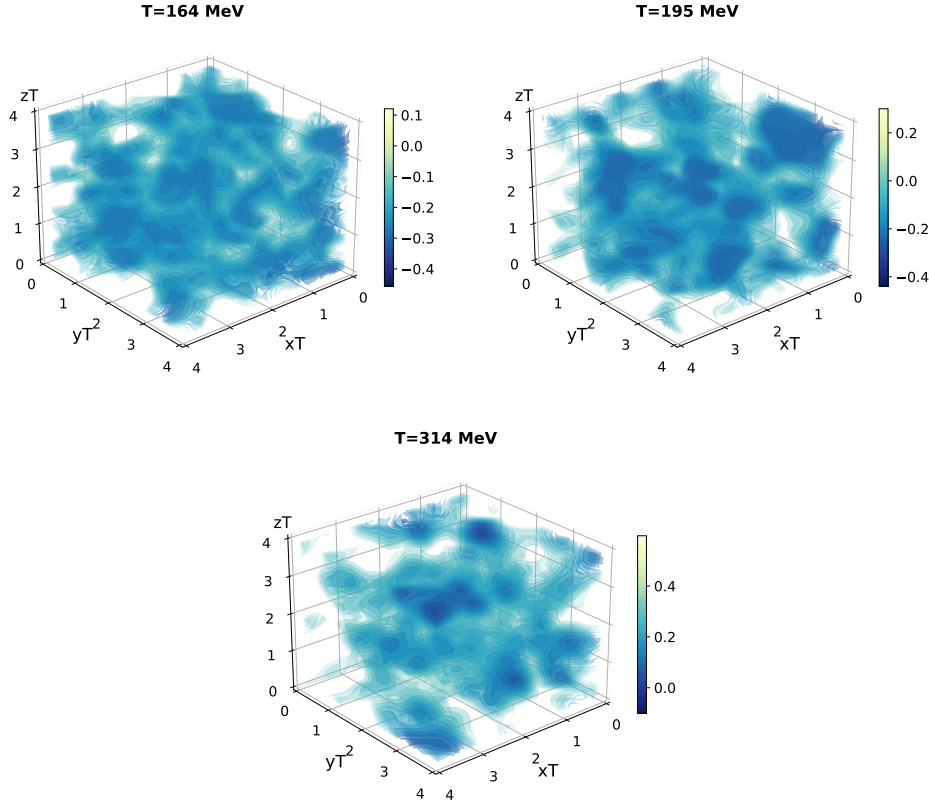


Figure 4.12: Visual representation of the local fluctuations of the local values of the real part of the Polyakov loop $\text{Re}.P(\mathbf{x})$ which are below its mean value at three different temperatures obtained after performing Wilson flow renormalization in a typical configuration. The lightest color in the palette represents its mean value in that particular gauge configuration.

different temperatures superposed together in Fig. 4.11. We observe that the width of the distribution of the renormalized local Polyakov loop values is decreasing with increasing temperatures, demonstrating that the gauge fields are smoother at higher temperatures. Due to the larger width of the distribution at $T \leq 195$ MeV, the confining wells defined at locations in space for which the real part of the renormalized Polyakov loop values are lower than its average, have strong overlap with each other. This is also evident in the density plots of the local fluctuations of the Polyakov loop which are lower than its mean value at three different temperatures, shown in Fig. 4.12. At higher temperatures $T = 314$ MeV the large negative fluctuations in $\text{Re}.P(\mathbf{x})$ about its average value becomes rarer, resulting in a clear separation among these potential wells which are located at random sites. In contrast, close to the crossover transition at $T = 164$ MeV, the fluctuations in the

renormalized values of the Polyakov loop are much more frequent and correlated.

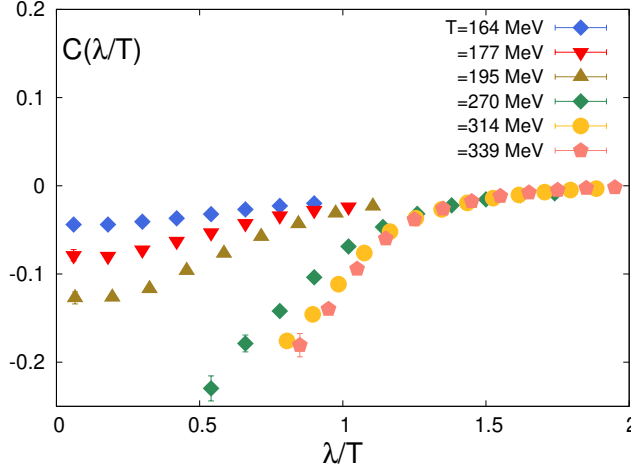


Figure 4.13: The correlation $C(\lambda/T)$ between the local density of the Dirac eigenstate and the local fluctuations of $\text{Re}.P(\mathbf{x})$ about its mean calculated in small bins of λ/T at different temperatures.

In order to quantify how well these deep negative fluctuations of the renormalized Polyakov loop $\text{Re}.P(\mathbf{x})$ about its mean are correlated with the Dirac eigenstates at each temperature, we calculate the quantity $C_n = \sum_{\mathbf{x}} |\Psi_n(\mathbf{x})|^2 [\text{Re}.P(\mathbf{x}) - \langle \text{Re}.P(\mathbf{x}) \rangle]$. Here $\Psi_n(\mathbf{x})$ is the n^{th} eigenstate of the overlap Dirac operator and its norm at each spatial site $\mathbf{x}$ on the lattice is obtained by summing over the four-dimensional eigendensity along the temporal direction τ denoted as $|\Psi_n(\mathbf{x})|^2 = \sum_{\tau=0}^{N_\tau-1} |\psi_n(\mathbf{x}, \tau)|^2$. We calculate the net correlation $C(\lambda/T)$ by performing a binning of the C_n , calculated for each eigenstate labeled by n , in small bins in λ/T and performing an average over the gauge configurations for different temperatures, results of which are compiled in Fig. 4.13. From the figure it is evident that at higher temperatures $T > 250$ MeV, the eigenvalues in the *intermediate* region of the Dirac spectrum are more correlated with the wells arising due to fluctuating renormalized Polyakov loops as compared to temperatures $T \leq 195$ MeV. This demonstrates that indeed the fluctuations in $\text{Re}.P(\mathbf{x})$ acts as random disordered confining potentials for these low eigenmodes at high temperatures, nonetheless it will be important to confirm this on a larger volume. At $T \leq 195$ MeV, the correlation between *intermediate* Dirac eigenstates with the local Polyakov loop fluctuations is weaker compared to temperatures $T > 250$ MeV. This is due to the fact that these well-like fluctuations at different lattice sites are no

longer rare events; on the contrary they are strongly correlated as observed in Fig. 4.11. As a result, the *intermediate* eigenstates are delocalized over several such locations. This was also evident from the spectral properties [72] and fractal-like structure [73] of these *intermediate* eigenstates at $T < T_{U(1)}$, discussed in the next section. The values of $C(\lambda/T)$ approach to zero for the bulk eigenstates, as expected, since these are delocalized chaotic states that do not feel the tiny local fluctuations in the renormalized Polyakov loop values.

4.6 Physical implications of our findings

Having categorized the infrared region of the Dirac eigenspectrum in terms of *intermediate* and bulk eigenmodes based on their distinct properties we now discuss some of the physical consequences of them.

4.6.1 *Intermediate* eigenmodes near T_{pc} and $U_A(1)$ breaking

In the previous Subsection 4.3.2 we have already discussed the different localization properties of *intermediate* and bulk eigenmodes in Fig. 4.4 quantified in terms of IPR D_2 for temperatures near T_{pc} . To understand the physical origin we now calculate the distribution of the fractal dimension D_f of the eigenvectors, in the same eigenvalue intervals where IPR was calculated. This is because the IPR is comparatively more noisy due to low statistics. However both of these quantities contain equivalent information about the scaling of the eigenmodes. We have calculated the fractal dimension of an eigenstate using the box-counting method [172] where the threshold for the probability density is chosen to be $0.75/V$. This choice yields a scaling behavior for D_f that is consistent with D_2 within errors across all λ/T bins. The probability distribution of the fractal dimensions $P(D_f)$ shown in Fig. 4.14, has been constructed using an error-weighted Gaussian smearing method, where the data is extracted from a Gaussian distribution centered at each measured value of D_f with a width given by its error. These data are summed and nor-

malized such that the area under the curve is unity, thus producing a smooth probability distribution function instead of discrete histograms. As evident from Fig. 4.14, the fractal dimensions of the bulk eigenmodes for all temperatures are significantly higher than the *intermediate* eigenmodes, the median values ranging between $2.78 \lesssim D_f \lesssim 2.84$. For the temperature range $\gtrsim T_{pc}$, the D_f of the *intermediate* eigenvectors show a sensitivity to temperature variation thus reflecting the physical changes occurring in the system due to the chiral crossover transition. The probability distribution of D_f has a spread due to the fact that fluctuations can exist on all length scales larger than the lattice spacing resulting in wavefunctions with different extent of delocalization to co-exist [173], with median values $D_f = 2.52, 2.49, 2.52, 2.55$ at $T = 164, 177, 186, 195$ MeV respectively. The median values of D_f of the critical modes near a phase transition can be interpreted using the relation $D_f = 3 - \beta/\nu$ [174]. If we put in the critical exponents β, ν of a three-dimensional O(4) spin model [175], the value of $D_f \simeq 2.485$ is similar to the median values of D_f observed for the *intermediate* eigenmodes just above the thermal crossover transition.

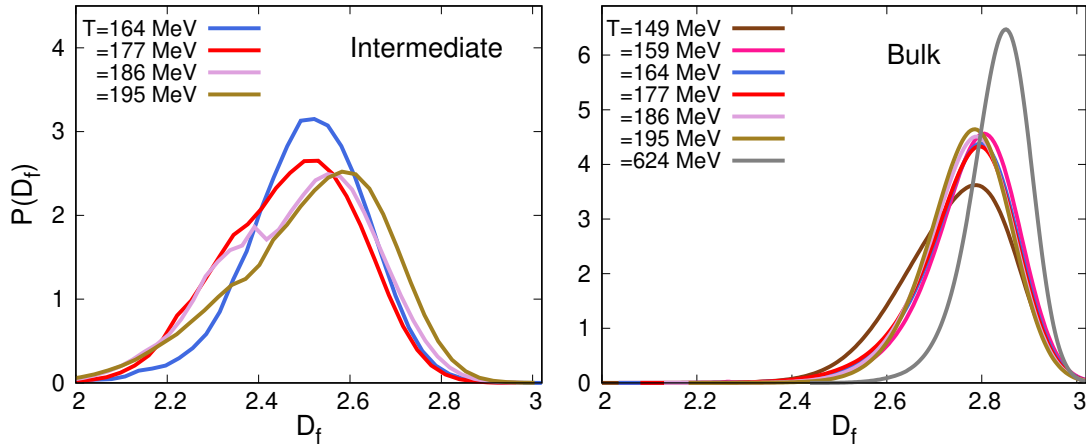


Figure 4.14: Probability distribution of the fractal dimension D_f at different temperatures and in eigenvalue intervals characterized as the *intermediate* (left panel) and the bulk eigenmodes (right panel).

The presence of small kinks in $P(D_f)$ at $T \gtrsim 186$ MeV is expected due to the rare occurrence of near-zero modes at high temperatures, hence one would require larger statistics to obtain a smooth curve. One also observes a spread of $P(D_f)$ towards lower values of $D_f \simeq 2$ with increasing temperatures, indicating the appearance of more localized ei-

genmodes. With this trend we expect that at even higher temperatures, localized eigenmodes characterized by $\langle \tilde{r} \rangle$ close to the value in a uncorrelated Poissonian distribution would contribute significantly to the broadening of $P(D_f)$. This can be related to the observation of an Anderson-Mott transition and the existence of a mobility edge at high temperatures [63, 85, 86, 88, 89, 176–181]. Eventually the low-lying eigenstates near or below the mobility edge, will exhibit a median value of fractal dimension similar to that in a 3-dimensional Anderson model [179]. At higher temperatures $T > T_{U(1)}$ we do not yet observe any signal of a Anderson-Mott like transition from the $\langle \tilde{r} \rangle$ data in Fig. 4.1. This might be happening because of the small physical volumes at these temperatures and hence requires a careful study in the thermodynamic limit. But we do see its signature in the correlation of the eigenstates with the real part of the Polyakov loop studied in Section 4.5.

We end this section by re-iterating again the fact that the *intermediate* Dirac eigenmodes appearing just above T_{pc} are fractal-like. Even though the chiral transition in QCD with physical quark masses is a smooth crossover, the fractal dimensions of the *intermediate* eigenmodes still carry the remnant information of the criticality, which could be $O(4)$ universality class. This also indirectly confirms that the $U_A(1)$ remains broken just above T_{pc} . The $O(4)$ universality is also supported from other independent lattice studies on the scaling of the order parameter in the chiral limit [18, 182]. Moreover the *intermediate* eigenmodes are prominently detectable in a temperature range where there are proposals of an IR conformal phase [70–72, 75, 76, 183, 184], appearance of emergent symmetries [185] and their eventual disappearance can explain the *effective* restoration of $U_A(1)$ subgroup of chiral symmetry [69]. We note here that the connection between phase transitions and fractals has also been discussed in the context of spin systems, e.g., in the Ising model [186] and in gauge theories without dynamical quarks [187, 188].

4.6.2 *Intermediate eigenmodes above $T_{U(1)}$ and localization*

As already discussed in the previous Subsection 4.6.1 the *intermediate* eigenmodes just above the chiral crossover transition carry information about the universal critical exponents which are typically extracted from the scaling of the order parameters in the chiral limit. However as higher temperatures $T < T_{U(1)}$ these *intermediate* eigenmodes have a very different physical origin.

One such quantity that can help us to distinguish between the *intermediate* Dirac eigenmodes in regimes $T < T_{U(1)}$ and above is Thouless conductance. It can be defined in terms of the curvature K_i acquired by the i -th eigenstate subject to an infinitesimally small twist as $g_{\text{Th}} = \frac{1}{\langle s \rangle} \langle K_i \rangle_{\eta \rightarrow 0}$. The curvature K_i for the i -th eigenmode is defined in a previous section of this chapter in Eq. 4.2. Calculating the averages of the curvatures $\langle K_i \rangle$ and level spacings $\langle s \rangle$ in small bins in λ/T for four different temperatures, we summarize our results for g_{Th} in Fig. 4.15. The initial growth in the values of the Thouless conductance as a function of λ/T in the bins containing *intermediate* eigenvalues is different compared to the bulk modes. Thus g_{Th} allows us to unambiguously disentangle the bulk eigenvalues from the rest. The g_{Th} are not insignificantly small for bins in the *intermediate* region, which implies that these eigenstates are not exponentially localized. Performing a fit to the data for bulk eigenvalues with a linear in λ ansatz, shown as dashed lines in Fig. 4.15, we obtain similar positive slopes $dg_{\text{Th}}(\lambda/T)/d(\lambda/T)$ for all four different temperatures.

Next, we focus only on the lowest few *intermediate* eigenvalues, which are strongly correlated with the gauge field fluctuations, quantified in terms of $C(\lambda/T)$. The results for Thouless conductance due to these *intermediate* eigenmodes as a function of temperature are shown in Fig. 4.16. It is clear that with increasing temperatures, the lowest few eigenmodes that are well localized within the wells formed due to fluctuations in the $\text{Re}.P(\mathbf{x})$ contribute to the Thouless conductance, thus lowering its magnitude. The values of g_{Th} at the highest two temperatures saturate, albeit with large errors due to an insufficient

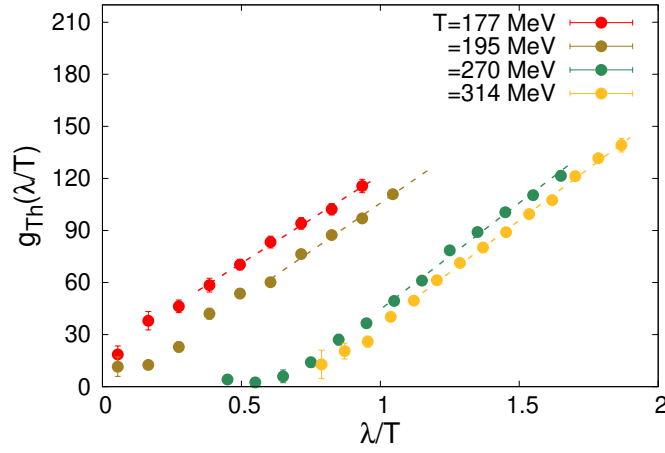


Figure 4.15: The Thouless conductance for different eigenvalue bins calculated at temperatures $T = 177, 195, 270, 314$ MeV respectively. The dashed line represents a linear fit to the $g_{Th}(\lambda/T)$ for bulk eigenmodes.

number of eigenmodes in the lowest bins and possibly finite-volume effects. However, the values of g_{Th} are significantly larger for $T < T_{U(1)}$ and grows with decreasing temperatures. Thus, the temperature dependence of g_{Th} allows for its potential use as an *order parameter* for the restoration of $U_A(1)$. Since $U_A(1)$ is not an exact symmetry, one cannot construct an order parameter for it within the Landau theory of phase transitions. Instead, we suggest that the effects of $U_A(1)$ breaking and restoration should be inferred from the change in the structural properties of the eigenstates, which are manifest in quantities like g_{Th} .

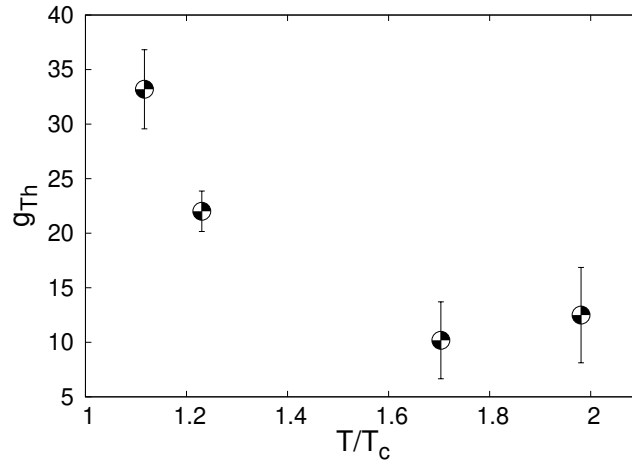


Figure 4.16: Thouless conductance for the smallest eigenmodes chosen such that these have similar values of $C(\lambda/T)$, shown as a function of temperature.

4.6.3 Bulk eigenmodes and approach to thermalization

At high temperatures much above the chiral crossover in QCD, the dominant degrees of freedom below the magnetic scale $g^2 T / \pi$ are gluons. We thus calculate $\langle \tilde{r} \rangle$ for the overlap Dirac eigenvalues at a temperature ~ 624 MeV, which is twice the deconfinement temperature, on SU(3) gauge configurations without dynamical quarks. All eigenmodes below the magnetic scale have values of $\langle \tilde{r} \rangle$ consistent with the prediction from RMT belonging to the GUE class. The average value of $\langle \tilde{r} \rangle$ for the eigenmodes is shown as a red point in the left panel of Fig. 4.2 and their probability distribution $P(r)$ is shown in the right panel of the same figure. The first Rényi entropy content due to the eigenmodes, their IPR, and fractal dimensions are shown in Fig. 4.4 and Fig. 4.14 respectively, confirming that indeed all the eigenmodes are delocalized over the entire volume and thus ergodic. Spectral properties of the Dirac eigenmodes in SU(3) gauge theory at $T \sim 624$ MeV indicate the chaotic nature of such a system.

Bohigas, Giannoni and Schmit (BGS) conjectured that [24] the universal quantum fluctuations of level-spacings between the energy eigenvalues of a system whose classical dynamics is chaotic can be described in terms of one of the three distinct Wigner classifications of RMT. Since a thermal state in QCD at high temperature exhibits spectral properties corresponding to a RMT, we would like to investigate if there exists a classical state that exhibits chaos. This will allow us to verify the BGS conjecture for this strongly interacting many-body system described by QCD.

Inspired by the Color Glass Condensate effective theory description of QCD [189], we construct a classical state of the non-Abelian SU(3) gauge theory where the gluons have an initial phase-space distribution,

$$g^2 f_g(|\mathbf{p}|, t = 0) = n_0 \frac{Q}{|\mathbf{p}|} e^{-\frac{|\mathbf{p}|^2}{2Q^2}}. \quad (4.3)$$

Here Q denotes the gluon saturation scale and $Q \gg \Lambda_{\text{QCD}}$, the typical confinement scale

in QCD. This initial state is clearly athermal and represents a typical state of QCD with an over-occupied infrared spectrum due to gluons whose occupation numbers $\sim n_0/g^2$ are non-perturbatively large since $g \ll 1$ [141]. Such a state is inherently classical. Starting with this initial condition, a classical Hamiltonian evolution of the gauge links $U_{i,\mathbf{x}}$ and its conjugate momenta i.e. electric fields $E_{a,\mathbf{x}}^i$ in time according to the equations of motion

$$\frac{\partial U_{i,\mathbf{x}}}{\partial t} = \frac{\partial H}{\partial E_{i,\mathbf{x}}}, \quad \frac{\partial E_{i,\mathbf{x}}}{\partial t} = -\frac{\partial H}{\partial U_{i,\mathbf{x}}}, \quad i = 1, 2, 3. \quad (4.4)$$

leads to a non-thermal fixed point for the momentum distribution function for gluons [142]. For such classical systems we can generalize the notion of chaos manifesting itself through the exponential separation with time t of two infinitesimally close trajectories at $t = 0$. This can be done by constructing of a gauge-invariant distance measure [190] defined as

$$D(t) = \frac{1}{N_P} \sum_P \frac{1}{N_c} \left| \text{tr} U_P - \text{tr} U'_P \right|, \quad (4.5)$$

in terms of the difference between expectation values of the plaquettes U_P and U'_P at time t which are infinitesimally close at $t = 0$. The trace is performed over the color degrees of freedom. In our calculations such an initial condition is set by tuning the gluon densities as n_0 and $n_0 + \Delta n_0$, where we have chosen $n_0 = 0.4-1.0$ and $\Delta n_0 = 0.001$. We then calculate the distance measure $D(t)$ as a function of time, the details of which are mentioned in Ref. [73] and also in the Ph. D. thesis of Harshit Pandey [191]. In summary, the main finding that is relevant for my thesis is that the $D(t)$ increases exponentially with time, eventually saturating at later times due to finite gauge-space volume. A positive Lyapunov exponent characterizing this exponential growth of the distance measure $D(t)$ was extracted for all the different initial conditions that we have studied. With this study we could show the existence of classical states in SU(3) which exhibit chaotic behavior and thus a non-trivial realization of the BGS conjecture in strongly interacting gauge theories. This has important implications for how fast the non-perturbatively interacting gluons, whose momenta are below the magnetic scale thermalize, details of which are in

Harshit Pandey's thesis [191].

4.7 Summary and outlook

In this chapter, we discuss our lattice studies on the properties of infrared eigenstates of the massless Dirac operator on thermal gauge ensembles, in order to understand the high-temperature phase of a strongly correlated system described by QCD. We particularly focused on the questions: how can we identify the *effective* restoration of the anomalous U(1) subgroup of chiral symmetry using spectral and structural properties of the Dirac eigenstates and what are its physical consequences. We have performed our calculations with an extensive set of gauge configurations generated using Möbius domain wall fermion discretization, over a range of temperatures up to $\sim 2 T_{pc}$. Using normalized level spacing ratios of eigenvalues of massless 1-particle states realized using the overlap Dirac operator, we could unambiguously identify eigenmodes which have *intermediate* level statistics and distinguish them from the overwhelming majority of the bulk eigenstates. These bulk eigenstates have level repulsions consistent with random matrices belonging to a GUE. We could demonstrate a non-trivial realization of the BGS conjecture for QCD at high temperature in terms of these bulk eigenstates.

We provide an explanation for the existence of these Dirac eigenstates with *intermediate* level statistics within a matrix model. By introducing additional uncorrelated eigenvalues within a large random matrix belonging to a GUE with a very specific accept/reject criterion, we showed that the normalized level ratios of this enlarged matrix, can beautifully explain *intermediate* level ratios of the QCD Dirac eigenvalues shown in Fig. 4.9. We also discussed an intuitive understanding of such a matrix model construction in terms of a Brownian model describing the dynamics of the eigenvalues. By studying the correlation of these *intermediate* eigenstates with fluctuations of the real values of the renormalized Polyakov loop about its average, we could clearly show their distinct physical properties

at high temperatures $T > 250$ MeV, where the axial $U(1)$ symmetry is expected to be effectively restored compared to $T < 200$ MeV, where it remains broken. In the temperature regime where $U_A(1)$ remains broken, the fractal dimensions of these *intermediate* eigenstates carry information about the universality class of the chiral phase transition. At higher temperatures $T > 250$ MeV the density plots for the real part of the renormalized Polyakov loop reveal the existence of deep localized fluctuations at random sites on the lattice which are uncorrelated with each other, mimicking random disorder as discussed in the context of the Anderson model of electrons. Although it is important to study the finite volume effects more carefully to understand whether these infrared eigenstates with *intermediate* level ratios describe the physics near the mobility edge in an Anderson-like transition. We also showed that fluctuations in the real values of the renormalized Polyakov loop below its mean at different lattice sites are strongly correlated at $T < 200$ MeV, quite unlike the original proposal of a random disorder by Anderson. Our study shows that localization of the most infrared Dirac eigenstates will start to become more prominent when the axial $U(1)$ subgroup of chiral symmetry is effectively restored.

We also, for the first time, calculate the analogue of the Thouless conductance g_{Th} in terms of the Dirac eigenstates which quantifies the structural rigidity of the different eigenstates due to a twist applied along one of the spatial boundaries of the lattice box. We use the curvature distribution and the g_{Th} to also independently distinguish between the *intermediate* eigenstates and the bulk. Calculating the g_{Th} for the *intermediate* eigenstates that are strongly correlated with the local Polyakov loop fluctuations, we demonstrate its gradual decrease as a function of temperature. The point of inflection of this curve could give us an estimate of the temperature where $U_A(1)$ is *effectively* restored, thus acting as an *effective* order parameter.

Chapter 5

Conclusions and Outlook

The research presented in this thesis uses the eigenvalue spectrum of the quark Dirac operator as the fundamental microscopic tool to understand the thermal phase structure of QCD. By systematically analyzing the eigenvalue density, nearest neighbor level spacing statistics, and spatial localization of these eigenmodes using different fermion discretizations on the lattice, we have provided rigorous, first principles results. Although the study of the Dirac eigenspectrum for understanding effective restoration of different subgroups of the nearly exact two-flavor chiral symmetry in QCD, my thesis provides some new perspectives in this vibrant but challenging field of research.

In Chapter 2 of my thesis, I address different issues related to the effective restoration of the anomalous $U_A(1)$ subgroup of chiral symmetry in QCD. I have used the highly improved staggered quark discretization on the lattice for this part of my work. By carefully performing a continuum extrapolation of the difference between integrated iso-triplet, scalar, and pseudo-scalar meson correlators, we could show that $U_A(1)$ remains broken even though the non-singlet subgroup of chiral symmetry is effectively restored. These correlators were calculated in terms of the Dirac eigenvalues, hence we could identify the microscopic mechanism behind this strong breaking of $U_A(1)$. The key observation arising out of my work is that as long as the peak-like accumulation of small eigenvalues

strongly overlaps with the bulk eigenspectrum, a non-trivial breaking of $U_A(1)$ symmetry persists. We could also show that the near-zero peak starts to get disentangled from the bulk eigenvalues at $T \sim 1.15 T_{pc}$ where the characteristic temperature dependence of relevant meson (integrated) correlators responsible for the non-trivial breaking of $U_A(1)$ also vanishes.

The robustness of these conclusions was further tested in Chapter 3, where the meaning of *effective* restoration of an anomalous symmetry, here, $U_A(1)$ was discussed. We went from the staggered discretization to utilize the good chiral and topological properties of Möbius domain wall fermions (MDWF). The later preserve chiral symmetry almost exactly, even on a finite lattice. However, the good chiral properties come with a formidable computational cost in generating dynamical gauge ensembles with MDWF. We discuss some efficient algorithmic optimizations— a careful choice of Hasenbusch masses for preconditioning [123] the light quark Dirac operator and the use of multi-step integrators for quarks and gauge links for an efficient sampling of gauge ensembles within a rational hybrid molecular dynamics algorithm. These optimizations allowed for a 20-40% increase in the throughput of generation of statistically independent gauge ensembles, just near the chiral crossover transition.

We also demonstrated in the same chapter that this extensive set of gauge configurations with MDWF discretization for quarks explored different topological sectors quite efficiently. As a consequence, topological charge fluctuations on a finite lattice cut-off, quantified in terms of topological susceptibility χ_{top} , are compatible with the continuum extrapolated results obtained with HISQ discretization for $T > T_{pc}$. Furthermore, temperature dependence of $\chi_{top}^{1/4}/T_{pc}$ at $T > T_{pc}$ can be characterized in terms of an exponent α as $(T/T_{pc})^{-\alpha}$. By monitoring the temperature dependence of α , we observe that at $T \lesssim 1.2T_c$ the value of α is not consistent with ~ 2 which is known from a dilute instanton gas model for $N_f = 3$. Only when χ_{top} is characterized by an exponent predicted from dilute gas of instantons one can infer about an *effective* restoration of $U_A(1)$. The observation of

a different exponent implies that the QCD vacuum between T_{pc} and $1.2 T_{pc}$ is still characterized by a strongly correlated gas of instantons. This was also observed from the non-trivial probability distribution of the lowest eigenvalue of the QCD Dirac operator in Chapter 2. The effective restoration of the non-singlet subgroup of chiral symmetry can also be inferred indirectly from the temperature dependence of χ_{top} . The fact that there exist a 50% deviation in χ_{top} values at $T \gtrsim 1.2 T_{pc}$ compared to its value calculated within NLO SU(2) chiral perturbation theory, is an indirect manifestation of the restoration of the SU_A(2) subgroup of two-flavor chiral symmetry in QCD.

In Chapter 4 of my thesis, I discuss the more microscopic properties of the Dirac eigenstates and try to interpret them in the context of sequential restoration of subgroups of the almost exact two-flavor chiral symmetry in QCD. Furthermore, we show how features of localization can be observed from the level spacing ratios of the most infrared eigenvalues only when U_A(1) is effectively restored. This led to our proposal that since U_A(1) is an anomalous symmetry that lacks a standard order parameter, structural changes of the Dirac eigenstates manifested in terms of Thouless conductance can provide the most reliable and physically motivated measure of its effective restoration.

Going back to our discussions on the *intermediate* eigenvalues of the QCD Dirac operator, we show that their normalized level ratios $\langle \tilde{r} \rangle$ are intermediate between the predictions from an uncorrelated Poisson ensemble and a random matrix ensemble consisting of Gaussian unitary matrices. We have formulated a matrix model to explain the probability distribution of $\langle \tilde{r} \rangle$ for these intermediate eigenmodes. This matrix model has a very nice theoretical interpretation in terms of Dyson's construction, which treats eigenvalues of random matrices as a gas of particles subject to a logarithmic repulsion and an attractive potential of simple harmonic oscillator type. We showed that choosing a weak confining potential of the type $V(\{\epsilon_i\}) \sim \sum \ln^2 |\epsilon_i|$ naturally produces the normalized spacing ratios observed in our lattice calculations, providing a universal description of the transition between ergodicity and localization.

Furthermore, we demonstrated that the physical origin of these *intermediate* eigenmodes depends crucially on the temperature. Just above T_{pc} , these eigenmodes have a median fractal dimension $D_f \approx 2.5$, which can be interpreted in terms of the two independent critical exponents of the 3D $O(4)$ spin model. This suggests that these *intermediate* eigenmodes carry a remnant of the universality class of chiral phase transition, even for physical quark masses. As the temperature is increased beyond 250 MeV, where $U_A(1)$ symmetry is effectively restored, the intermediate Dirac eigenstates become increasingly trapped within potential wells formed due to deep negative fluctuations in $\text{Re}P(\mathbf{x})$. Hence, these eigenmodes represent a scenario similar to an Anderson model near the mobility edge, but for a strongly interacting many-body system.

Finally, we showed an explicit realization of the Bohigas-Giannoni-Schmit (BGS) conjecture [24] in a non-perturbatively interacting quantum field theory, here $SU(3)$, in terms of the bulk Dirac eigenmodes. Whereas there exist classical states in $SU(3)$ which exhibit chaos, the Dirac eigenfunctions on quenched $SU(3)$ gauge configurations at $T \sim 600$ MeV have level ratios consistent with a GUE, thus demonstrating the validity of this conjecture.

The findings presented in this thesis open several broad areas for future inquiry. We have performed our study with a state-of-the-art overlap Dirac operator as a probe of our MDWF ensembles on a modestly large lattice size. The most immediate challenge is the precise determination of the mobility edge, which separates localized infrared eigenstates from delocalized bulk eigenstates in the thermodynamic limit. This will require large-scale simulations on larger spatial volumes to properly account for finite-size scaling and the potential emergence of a true mobility edge in the infinite volume limit. Furthermore, the fractal nature and non-ergodicity of the infrared eigenstates are suggestive of the many-body localization (MBL) phenomenon, which needs to be also verified in the thermodynamic limit. Additionally, the development of efficient integrators for MDWF will eventually allow for performing studies on significantly larger and finer lattices. This would enable us to explore even higher temperatures where we can study the transition

from a localized to a weak metallic phase. Ultimately, the integration of spectral analysis and localization phenomenon can deepen our understanding of the transport properties and the mechanism of thermalization in a strongly interacting nuclear matter described by QCD.

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