Exploring Jet Transport Coefficients In The Quark-Gluon Plasma

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EXPLORING JET TRANSPORT COEFFICIENTS IN THE QUARK-GLUON PLASMA

by

AMIT KUMAR

DISSERTATION

Submitted to the Graduate School
of Wayne State University,
Detroit, Michigan
in partial fulfillment of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

2020

MAJOR: PHYSICS

Approved By:

________________________
Advisor                      Date
DEDICATION

To my parents and sister, for their unconditional love and support
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CHAPTER 1 INTRODUCTION

Questions such as “What is the origin of the universe?” and “How the universe has evolved in time to what we see now?” have fascinated mankind for a long time. Much progress has been made in finding answers to these questions. Today, we know that our universe was created from an exploding hot and dense fire ball, called the big bang. Estimates tell us that within the first few microseconds of the Big Bang, the temperature of our universe was so high that quarks and gluons, which are usually bound inside conventional hadrons, existed in a deconfined state. This phase of matter is called the Quark-Gluon Plasma (QGP). As the universe expanded, the temperature decreased to $T \lesssim 160$ MeV [18], quarks and gluons could no longer exist in a free state and became confined to form hadrons. The QGP, which is only known to exist above $T \approx 160$ MeV, is now routinely created in high energy heavy-ion collisions at the Relativistic Heavy-Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) and the Large Hadron Collider (LHC) at the European Center for Nuclear Research (CERN).

1.1 QCD Lagrangian

Quantum Chromodynamics (QCD) is a quantum field theory that describes the strong nuclear force. It is a gauge theory where the quarks are in the fundamental representation of $SU(3)$ group. The quark field $\psi(x)$ under the operation of the group element $\Omega$ of the $SU(3)$ group, transforms in the following manner

$$\psi'(x) = \Omega(x)\psi(x), \quad \Omega(x) = e^{-iT^a\theta^a(x)},$$

where \(\Omega(x) \in SU(3)\) can be parametrized by a set of continuous parameters \(\theta^a(x)\). Here, the \(\theta^a\)'s are minimum number (sufficient) of real parameters to uniquely define the $SU(3)$ group elements and \(a\) runs from 1 to 8. The $T^a$'s are (Gell-Mann matrices) refered to as generators of the $SU(3)$ group and follow the Lie algebra \([T^a, T^b] = if^{abc}T^c\), where \(f^{abc}\) are completely antisymmetric structure constants of the $SU(3)$ group.
The QCD Lagrangian density for the free fermion field is given by

$$\mathcal{L}(x) = \bar{\psi}(x) [i\gamma^\mu \partial_\mu - m] \psi(x),$$  \hspace{1cm} (1.2)

where $\gamma^\mu$'s are the Dirac gamma matrices and $m$ is the mass of quanta of the fermion field. Applying the transformation 1.1 we can see that the Lagrangian density (Eq. 1.2) is invariant under the global transformation, i.e., when the parameters $\theta^a(x)$ are independent of the location $x$. However, for the transformation 1.1 in which the phase rotation angle $\theta(x)$ varies arbitrarily from point to point, the QCD Lagrangian is no longer invariant. The invariance under the local transformation is broken mainly due to the presence of the derivative term given as

$$\partial_\mu \psi(x) = \lim_{a \to 0} \frac{\psi(x + a\hat{\mu}) - \psi(x)}{a}. \hspace{1cm} (1.3)$$

In above Eq. 1.3, the two fermion fields to be subtracted, $\psi(x + a\hat{\mu})$ and $\psi(x)$, have different transformation properties. To circumvent this problem, we introduce the gauge link $U_\mu(x + a\hat{\mu}, x) \in SU(3)$ that depends on the two points and has the following transformation property

$$U'_\mu(x + a\hat{\mu}, x) = \Omega(x + a\hat{\mu})U_\mu(x + a\hat{\mu}, x)\Omega(x) \hspace{1cm} (1.4)$$

together with Eq. 1.1. We set $U_\mu(x, x) = 1.$

Now, the object $U_\mu(x + a\hat{\mu}, x)\psi(x)$ transforms in same manner as $\psi(x + a\hat{\mu})$, and hence, can be subtracted in a meaningful way. This property leads one to define a new form of the derivative, called the covariant derivative, given as

$$D_\mu \psi(x) = \lim_{a \to 0} \frac{\psi(x + a\hat{\mu}) - U_\mu(x + a\hat{\mu}, x)\psi(x)}{a}. \hspace{1cm} (1.5)$$

Since $D_\mu \psi(x)$ transforms in same way as $\psi(x)$, we can construct the kinetic term for fermions in the Lagrangian density as $\bar{\psi}(x)\gamma^\mu D_\mu \psi(x)$ which is invariant under local $SU(3)$ transformation (Eq. 1.1 and 1.4).
As the gauge link $U_\mu(x + a\hat{\mu}, x)$ is an element of the $SU(3)$ group, we can write it in terms of the Hermitian generators of the $SU(3)$ group. The most general expression in limit of infinitesimally separated points can be written as:

$$U_\mu(x + a\hat{\mu}, x) \equiv \lim_{a \to 0} e^{igaA_μ^a(x)t^a} = 1 + igA_μ^a(x)t^a + O(a^2),$$

(1.6)

where $g$ is the coupling parameter and $A_μ^a(x)$ is a new vector field. For $SU(3)$ gauge theory, we require 8 vector fields $A_μ^a(x)$, one for each generator of the group. The fields $A_μ^a(x)$ are an effective degree of freedom and interpreted as gluons.

Now, the covariant derivative can be re-written by substituting Eq. 1.6 into Eq. 1.5 as

$$D_\mu \psi = \lim_{a \to 0} \frac{\psi(x + a\hat{\mu}) - \psi(x)}{a} - igA_μ^a(x)t^a\psi(x) = \partial_\mu \psi(x) - igA_μ^a(x)t^a\psi(x).$$

(1.7)

This implies that the covariant derivative has following form,

$$D_\mu = \partial_\mu - igT^aA_μ^a(x).$$

(1.8)

To obtain the transformation property of the gauge field $A_μ^a(x)$, we do a Taylor expansion (Eq. 1.4):

$$1 + igA_μ^a(x)t^a + O(a^2) = \Omega(x + a\hat{\mu})(1 + igA_μ^a(x)t^a + O(a^2))\Omega^\dagger(x)$$

$$1 + igA_μ^a(x)t^a + O(a^2) = \left[1 + a\partial_\mu + O(a^2)\right]\Omega(x) \left(1 + igA_μ^a(x)t^a + O(a^2)\right)\Omega^\dagger(x)$$

(1.9)

$$t^aA_μ^a(x) = \Omega(x) \left[t^aA_μ^a - \frac{i}{g}\Omega^\dagger\partial_\mu\Omega\right]\Omega^\dagger + O(a).$$

Now, to construct a kinetic term consisting purely of the gauge fields, we consider com-
mutator of the covariant derivatives applied on the fermion field \( \psi(x) \). We obtain

\[
[D_\mu, D_\nu] \psi(x) = -ig (\partial_\mu A_\nu - \partial_\nu A_\mu - ig[A_\mu, A_\nu]) \psi(x) \quad (1.10)
\]

The quantity within the parenthesis is identified as the non-Abelian gauge field strength given as

\[
F_{\mu\nu} \equiv F^a_{\mu\nu} t^a = (\partial_\mu A^a_\nu - \partial_\nu A^a_\mu + gf_{abc} A^b_\mu A^c_\nu) t^a \quad (1.11)
\]

Using the above \( F_{\mu\nu} \), one can construct a gauge invariant kinetic term for the gauge fields, given as

\[
\text{Tr}[F_{\mu\nu} F^{\mu\nu}] = \frac{1}{2} F^a_{\mu\nu} F^a_{\mu\nu} \quad (1.12)
\]

Finally, the full QCD Lagrangian density that is invariant under the \( SU(3) \) local gauge transformations (Eq. 1.1 and Eq. 1.9) is written as

\[
\mathcal{L}(x) = \bar{\psi}(x) [i \gamma^\mu D_\mu - m] \psi - \frac{1}{4} F^a_{\mu\nu}(x) F^{a\mu\nu}(x), \quad (1.13)
\]

where the factor \(-1/4\) is accounted to recover classical equation of motion. The parameter \( g \) represents the coupling constant. The crucial feature of the non-Abelian gauge theory is that the Lagrangian contains the cubic and quartic terms in the form of a derivative of each of the gauge field. This means that the \( SU(3) \) gauge fields can interact with each other. It should be noted that the gauge fields are required to insure the local gauge invariance of the Lagrangian (Eq. 1.1).

Often, the Feynman diagrams calculated in QCD involve the quark self-energy, the vacuum polarization, the vertex corrections, and gluon-loop corrections graphs [19, 20]. In all such diagrams, one encounters an ultra-violet (UV) divergent integrals. To make the integrals mathematically manageable, one regulates the integral using procedure such as dimensional regularization [21, 24] or Pauli-Villars regulators method [25] etc. The elimination of the UV divergences requires a “renormalization” [19, 20] procedure in which the bare parameters
appearing in the Lagrangian are rescaled. In the renormalization procedure, the bare parameters such as coupling constant and the mass acquire a scale dependence \( \mu \) set by matching them to a measured value at a given scale. The running coupling constant is an effective coupling constant that depends on the scale \( \mu^2 \), which is the momentum transfer \( \mu^2 \) of the process. At one-loop renormalization, one can express the running QCD coupling constant \( (\alpha_s) \) and QCD beta function \( (\beta(g)) \) as

\[
\alpha_s(\mu^2) \equiv \frac{g^2(\mu^2)}{4\pi} = \frac{4\pi}{\left[11 - \frac{2N_f}{3}\right] \ln \left(\frac{\mu^2}{\Lambda_{\text{QCD}}^2}\right)}, \quad \beta \equiv \mu \frac{\partial g}{\partial \mu} = -\frac{g^3}{16\pi^2} \left[11 - \frac{2N_f}{3}\right].
\]

(1.14)

respectively. If the number of quark flavors \( N_f < 16 \) (nature only has 6), the \( \beta \) function is negative. This implies that the strong coupling constant decreases with increasing the momentum scale, and hence, QCD is asymptotically free at high energy. Physically, this is attributed to the anti-screening nature of the gluon, which themselves carry the color charge. In a vacuum, as one moves away from the test charge (quark), the virtual gluons from the vacuum polarization enhance the effective charge around the test charge. Thus, getting closer to the test charge would weaken the effective charge and the effective coupling. This basic property of QCD allows one to study various partonic processes using perturbative methods and involves expansion in terms of \( \alpha_s \) at relevant scale \( \mu \gg \Lambda_{\text{QCD}} \sim 200 \text{ MeV} \).

1.2 Phases of QCD matter

The quarks and gluons are fundamental degrees of freedom of nuclear matter and, under normal circumstances, are confined inside hadrons. However, at a sufficiently high temperature, the quarks and gluons are found in a deconfined state. The existence of the QGP was first predicted by Collins and Perry in Ref. [26] and subsequently by others in Ref. [27–29]. The plot in Fig. 1.1 suggests that when a nuclear matter is heated to a sufficiently high temperature, the entropy density \( (s) \) scaled by \( T^3 \) exhibits a rapid increase [12]. The sharp increase above \( T \sim 160 \text{ MeV} \) in \( s/T^3 \) is a characteristic feature of a transition from the hadronic phase to a QGP phase, in which new color degrees of freedom (quarks and gluons)
emerge. The horizontal arrow in the plot indicates the Stefan-Boltzman (SB) limits, in which the deconfined quarks and gluons are non-interacting. The deviation from the SB limit is due to residual interactions between the quarks and gluons in the QGP phase.

Figure 11: The energy density normalized by $T^4$ as a function of the temperature on $N_t=6$, 8, and 10 lattices. The Stefan-Boltzmann limit $\epsilon_{SB} = 3 p_{SB}$ is indicated by an arrow.

Figure 12: The entropy density normalized by $T^3$ as a function of the temperature on $N_t=6$, 8, and 10 lattices. The Stefan-Boltzmann limit $s_{SB} = 4 p_{SB}/T$ is indicated by an arrow.

Now, in Fig. 1.2, we show an anticipated region of three possible phases (hadron gas, quark-gluon plasma, and color superconductor) of QCD matter in terms of the control parameters temperature $T$ and baryon chemical potential $\mu_B$. The bottom left region of the phase diagram where $T$ and $\mu$ are both small, the nuclear matter is in the hadronic phase, a composite state of quarks and gluons. As the temperature and the baryon chemical potential are increased, there comes a point where either a transition or a crossover occurs to a deconfined phase of quarks and gluons. The phase transition along the $\mu = 0$ is a cross over rather than a true phase transition, with a possibility of a critical point at the end of a line of the first-order transition.

At a fixed temperature, as one increases $\mu_B$ to a sufficiently high value, another kind of phase transition is believed to occur in which quarks rather than nucleons are the dominant degrees of freedom. Such extreme conditions may conceivably be found at the cores of
highly dense astrophysical objects such as neutron stars \cite{26}. It has been also speculated that the system could be in a state of color superconductor where phenomenon analogous to superfluidity in liquid $^3$He and superconductivity in metals arise.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{phase_diagram.png}
\caption{The phase diagram of nuclear matter \cite{3}.}
\end{figure}

In the next section, we discuss how the QGP is produced in relativistic heavy-ion collisions.

1.3 Stages in heavy-ion collision

In experiments such as RHIC and LHC, heavy-ions (such as gold or lead) are stripped of their electron cloud and then accelerated to high-energy and made to collide. The Fig. \ref{fig:1.3} and \ref{fig:1.4} show the different stages of a heavy-ion collision. In each heavy-ion collision event, the two ions collide with an impact parameter ($b$) which is defined as the shortest distance between the centers of the two colliding nuclei during the course of the collision (to the extent that centers may be defined for a given state of a nucleus). We define the reaction plane as a plane consisting of the impact parameter and initial beam direction ($z$-axis). The two nuclei moving at relativistic speeds are compressed to disks due to the Lorentz contraction. Unlike
the case of proton-proton (p-p) collisions, where a few particles are produced, almost free of one another, the tremendous amount of stopping that takes place in a heavy-ion collision leads to the formation of a dense interacting system. The strong interactions among the constituents in this system lead to thermalization and the formation of the QGP. The QGP, being a thermalized system, expands under its own pressure. This rapid expansion leads to the cooling of the expanding plasma. It should be noted that the QGP, on thermalization, is only locally (not globally) thermalized, i.e., there is a temperature gradient from the hot center of the system to the exterior vacuum. The expansion of the locally thermalized system can be described using the equations of relativistic viscous hydro-dynamics \[30-34\]. Later when the energy density of the QGP reaches \( e_{cr} \sim 1 \text{ GeV/fm}^3 \) \[35, 36\], the plasma undergo a phase transition. Below this density, the QGP cools back to a plasma of hadrons. The hadronic plasma continues to cool further. Between a temperature from 160 MeV to 120 MeV, hadrons in the plasma tend to progressively decouple from the medium. Eventually, these freeze out from the surface of the fireball and free stream to the detectors.

The QGP formed in such collisions cannot be directly accessed by the detectors. The properties of the QGP can only be discerned by studying the debris of hadrons hitting the detectors, that are placed at predetermined locations along with the accelerator where collisions take place. In the next section, we discuss how high-transverse momentum particles (high-\( p_T \)) can be used to study properties of this exotic state of matter.

![Figure 1.3: Stages in heavy-ion collision at RHIC and LHC (Ref. [4]).](image)
sections. Therefore, the cross-sections for hard-scattering processes should scale with the number of binary nucleon-nucleon collisions. Perfect liquid hydrodynamics suggest that initial anisotropy in the coordinate space are directly converted into the momentum anisotropy in the final momentum space. Since hydrodynamic model always assumes the local thermal equilibrium, the relation between initial spatial eccentricity and the final momentum anisotropy could provide the signal of possible thermalization in the early stage of heavy ion collisions.

1.2.2 Time Evolution

Figure 1.4: The space-time evolution of a heavy-ion collision [5].

1.4 High-\(p_T\) jets as a probe of the QGP

Jets are an important tool to study the properties of the QGP matter. Jets are highly collimated sprays of particles carrying high-transverse momentum (transverse to the beam). They are generally produced back-to-back (sometimes three or four jet events also occur) during the early stage of the collision. The partons produced from the hard scattering tend to undergo collinear radiation. Jets produced at the earliest stages in the collision of heavy-ions, have to traverse a portion of the medium prior to escape from the QGP. In the process of burrowing through the plasma, the jets are modified by the medium. For example, it can be argued (in the average event) that jets produced at the edge of the QGP fireball can escape easily (defined as trigger jet), while the jet emitted azimuthally opposite to it, will traverse a longer length through QGP medium, and on average will undergo significant energy loss compared to the other jet.

The Fig. 1.5 shows the back-to-back di-hadron correlation functions from \(Au + Au\)
collisions at $E_{cm} = 200$ GeV compared to $p$-$p$ collision [6]. We can clearly see that for $Au + Au$ collision, the correlated hadron yield has not changed much on the near-side, but has strongly suppressed on the away side. Since, $p$-$p$ collisions do not, on average, produce a QGP medium, one can take this as a reference to compare the yield of the particles produced in the $p$-$p$ collision with the particle yield in nucleus-nucleus collision, and study how the hard partons are modified by the medium.

![Graph of centrality dependent back-to-back di-hadron correlation functions](image)

**Figure 1.5:** Comparision of centrality dependent back-to-back di-hadron correlation functions for $Au + Au$ collision at $E_{cm} = 200$ GeV with $p$-$p$ collision [6]. Here, $0 < |\Delta \eta| < 1.4$ and $1.4 < p_{T}^{trig} < 4$ GeV.

There are several observables which can be used to study jet quenching in the QGP medium. We define here two important observables: nuclear modification factor $R_{AA}$ (jet or single-hadron) and hadron (jet) azimuthal anisotropy $v_2$. The $R_{AA}$ measures the high-$p_T$
hadron (jet) yield relative to the expectation from the $p$-$p$ collisions scaled by the number of expected binary collisions in a nucleus-nucleus collision, i.e.

$$R_{AA} = \frac{d^2N_{AA}(b_{\text{min}}, b_{\text{max}})/dyd^2p_T}{<N_{\text{bin}}(b_{\text{min}}, b_{\text{max}})>d^2N_{pp}/dyd^2p_T},$$

(1.15)

where $p_T = \sqrt{p_x^2 + p_y^2}$ is transverse momentum (beam is in $z$-direction), rapidity $y = (1/2) \ln [(E + p_z)/(E - p_z)]$, $d^2N_{AA}(b_{\text{min}}, b_{\text{max}})$ is the differential yield of hadrons (jets) in bins of $p_T$, rapidity $y$, and centrality $[b_{\text{min}}, b_{\text{max}}]$ for nucleus-nucleus collision, $d^2N_{pp}$ is differential yield of hadrons (jets) in $p$-$p$ collision, $<N_{\text{bin}}(b_{\text{min}}, b_{\text{max}})>$ represents average binary collisions in a nucleus-nucleus collision in centrality bin $[b_{\text{min}}, b_{\text{max}}]$. If quenching were present, the above ratio would be less than unity.

Jet quenching is length-dependent, and in a spatially anisotropic medium, quenching could change the azimuthal pattern of the particle distribution. This effect is called azimuthal anisotropy and is quantified in terms of azimuthal Fourier coefficients of the transverse momentum spectrum of the particles:

$$R_{AA}(p_T, \phi) = R_{AA}(1 + 2v_2\cos(2\phi - 2\psi) + ...),$$

(1.16)

where $\phi$ is the azimuthal angle and $\psi$ is the reaction plane angle. Reflection symmetry with respect to the reaction plane forbids the appearance of sine terms in the above expansion.

In this thesis, we will mainly focus on single-hadron and inclusive-jet observables, and leave other jet observables for future work.

1.5 Kinematic variables in relativistic heavy-ion collisions.

In this section, we review the basic kinematic variables used in the study of relativistic heavy-ion collisions. They possess simpler transformation properties under Lorentz boosts and allow for easier calculations. For instance, consider the rapidity of a particle which is defined as

$$y = \frac{1}{2} \ln \left[ \frac{E + p_z}{E - p_z} \right] = \frac{1}{2} \ln \left[ \frac{1 + v_z}{1 - v_z} \right],$$

(1.17)
where \( v_z = p_z/E \) represents the z-component of the particle’s velocity. The rapidity defined above can take values from \(-\infty\) to \(\infty\). It is an additive quantity under Lorentz transformation of the coordinate system, and hence behaves as the Newtonian velocity in a non-relativistic context. For instance, if a particle has energy momentum \((E', p'_x, p'_y, p'_z)\) in a frame \(S'\) that is moving with velocity \(\tilde{v}_z\) w.r.t frame \(S\), then the rapidity in frame \(S'\) is given as

\[
y' = \frac{1}{2} \ln \left( \frac{E' + p'_z}{E' - p'_z} \right) = \frac{1}{2} \ln \left( \frac{\gamma(E - \beta p_z) + \gamma(p_z - \beta E)}{\gamma(E - \beta p_z) - \gamma(p_z - \beta E)} \right) = \frac{1}{2} \ln \left[ \frac{1 + \tilde{v}_z}{1 - \tilde{v}_z} \right] \Rightarrow y' = y + y_{S'S}.
\]

So, we instead of working with \((E, p_x, p_y, p_z)\), we can work with this new four-vector \((m_T, p_T x, p_T y, y)\), where \(m_T = \sqrt{E^2 - p_z^2}\) is transverse mass and \(p_T = \sqrt{p_T^2 + p_T^2}\) is transverse momentum. This new coordinate system is often called Milne coordinates. In this similar spirit, the regular Minkowski space-time can be represented in a Milne coordinates as follows

\[
(t, x, y, z) \rightarrow (\tau, x, y, \eta) = \left( \sqrt{t^2 - z^2}, x, y, \frac{1}{2} \ln \left[ \frac{t + z}{t - z} \right] \right).
\]

We refer \(\tau\) as a proper time, whereas \(\eta\) as a spatial rapidity.

Often the theoretical calculations in heavy-ion physics are complex and require simplifying assumptions to gain a deeper understanding of underlying physics. For instance, to describe the hydrodynamics expansion of the fluid following the collision, one can assume the longitudinal boost-invariance. Based on the flatness in the multiplicity distribution of particles, Bjorken in 1983 \[37\] argued that at high energies, the physics of secondary particle production should be independent of the rapidity (or the longitudinal reference frame). The flat region near the center in the multiplicity distribution viewed as a function of rapidity is referred to as the central-plateau region and has been observed fairly well in experiments \[38, 39\]. This means that the initial conditions of local observables are only a function of proper time \(\tau\) and independent of \(\eta\). Also, the boost-invariance of these initial conditions
is preserved if the fluid expands along the longitudinal direction with a specific velocity profile \(v_L = z/t\).

With this picture of Bjorken expansion, we show the space-time evolution of QGP in Fig. 1.4 where the nuclear collision occurs at \(z = 0\). The hyperbolas are the contours of the constant proper time \(\tau\), which in asymptotic limit becomes forward and backward light cones represented by the equation \(t = \pm \sqrt{z^2 + \tau^2}\). The contours of constant spatial rapidity would be lines passing through origin with slope \(t/z = \coth(\eta)\). At \(t=0\), the colliding nuclei deposit the energy in the region \(z = 0\), and the system undergoes a pre-equilibrium phase. It is only after the thermalization at initial proper time \(\tau = \tau_0\) (hyperbola), the QGP is formed. Then, the QGP undergoes a hydrodynamic expansion and followed by cooling. Finally, at a final proper time \(\tau_f\), the system undergoes hadronization and freezes out.

To describe high-energy scattering processes in a hadronic or lepton-hadronic collision, it is very common to use light-cone variables instead of Milne coordinates, which are well suited to study the bulk-dynamics of the QGP. The presence of ultra-relativistic particles and a preferred axis of the propagation in these collisions drives one to employ light-cone coordinates. In this system, the Minkowski coordinate \((X^0, X^1, X^2, X^3)\) can be written in terms of light-cone variable as follows:

\[
(X^0, X^1, X^2, X^3) \rightarrow (X^+, X^-, X^1_\perp, X^2_\perp) = \left(\frac{X^0 + X^3}{\sqrt{2}}, \frac{X^0 - X^3}{\sqrt{2}}, X^1, X^2\right).
\]  (1.20)

The scalar product of four-vectors \(p\) and \(q\) is defined as

\[
p \cdot q = p^+ q^- + p^- q^+ - p^1_\perp q^1_\perp - p^2_\perp q^2_\perp.
\]  (1.21)

It can be easily verified that the above quantity is a Lorentz invariant scalar product. One of the motivations to employ these coordinates is the transformation properties under Lorentz boosts along the \(z\)-direction. In this coordinate system, when a vector boosted along the
z-direction, the light-cone plus-component and minus-component exhibit a large separation in the magnitude. This allows one to do a power counting and extract the most dominant terms in the calculations.

1.6 Outline of thesis

The subsequent chapters of this thesis are organized as follows:

- Chapter 2 presents the central goal of the thesis.

- Chapter 3 presents a brief theoretical background of the higher-twist energy loss formalism. We shall discuss the fundamental properties of QCD and the notion of factorization in a heavy-ion collision, an important tool to study scattering processes in a high-energy limit. We shall outline salient features of the single-scattering-induced emission within the higher-twist energy loss formalism. In the end, we discuss the extension to a multiple emission formalism and establish the medium-modified DGLAP evolution equation. In this chapter, we will also review the work done by the JET collaboration.

- Chapter 4 will discuss our formalism of the scale-dependence of $\hat{q}$, which is a leading parameter that controls the transverse broadening of the hard parton. In this effort, $\hat{q}$ is reformulated and expressed for the first time in terms of the QGP-PDF using the tools of perturbative QCD (pQCD). We shall fold this new $\hat{q}(T, E, \mu^2)$ in the medium-modified DGLAP equation and perform a full-model numerical calculation. This proposed formalism provides the first successful extraction of QGP-PDF and resolution of the $\hat{q}$ JET collaboration puzzle, i.e., enhancement in the interaction strength $\hat{q}/T^3$ at RHIC relative to LHC collision energies.

- Chapter 5 presents a brief review of the basic elements of lattice QCD. We shall discuss the underlying concept in setting up fermions and gauge fields on quenched and unquenched SU(3) lattices.
Chapter 6 will present our lattice formulation of transport coefficient $\hat{q}$. We developed a state-of-the-art framework that allowed us to extract the temperature dependence of $\hat{q}$ using the lattice gauge theory. We shall present our estimates of the temperature dependence of $\hat{q}$ for pure gluon plasma and quark-gluon plasma cases.

Chapter 7 will discuss Monte-Carlo based study of jet quenching within the framework of JETSCAPE.

Chapter 8 will discuss the conclusion and outlook for the study carried out in the thesis.
CHAPTER 2  CENTRAL GOAL OF THE THESIS

The description of matter in terms of its elementary constituents quarks and gluons remains one of the big unsolved problems of elementary particle and nuclear physics. In such efforts, one of the goals is to extract the momentum distributions of relevant degrees of freedom (partons or quasi-particles) using the fundamental theory of strong interactions, quantum chromodynamics (QCD). In this regard, the proton is the most widely studied QCD system. At an energy scale of the order of $\Lambda_{\text{QCD}} \sim 200$ MeV, the quarks and gluons are subjected to confinement. At very high boost the interaction is slowed down to an extent that the partons may be thought of as quasi free. This latter property called “asymptotic freedom” has been successfully used to extract the proton’s structure from collision processes of protons with leptonic projectiles such as the electron.

Since an electron has a point-like structure and the electron-photon dynamics (QED) is well-understood, the electron provides a perfect probe to “see” the proton’s structure. To leading order in electromagnetic coupling $\alpha_{\text{em}}$, the scattering of the electron and the proton occur through the exchange of a virtual photon with off-shellness $q^2 = -Q^2$ (virtuality). For the case, where the photon’s virtuality is large, the proton fragments during the scattering and the process is generally referred to as Deep Inelastic Scattering (DIS). Using the Hadron-Electron Ring Accelerator (HERA), the experimental group at DESY Hamburg performed a series of inelastic ep scattering experiments from 1992-2000 (HERA Phase I) and 2002-2007 (HERA Phase II) which showed that the structure of the proton is a scale-dependent phenomenon [7]. The experiment was performed at high center-of-mass energy, $\sqrt{s} \simeq 320$ GeV, where $s = 4E_eE_p$, the lepton beam energy $E_e \simeq 27.5$ GeV and the proton beam energy $E_p = 920$ GeV for most of the running period.

The Fig. 2.1 represents the probability distribution of parton’s momentum fraction ($x$) for $Q^2 = 1.9$ GeV$^2$ and 10 GeV$^2$ extracted by the HERA group. Increasing the $Q^2$ leads to enhancement in the number of partons at low $x$ and suppression in the high $x$ region. At $Q^2 < 2$ GeV$^2$, the proton is predominantly consists of three valence quarks (uud). In high
$Q^2$ and low $x$ region, the virtual photon can resolve more and more quark-antiquark pairs produced from the quantum fluctuations inside the proton. They are called sea quarks. The fraction carried by gluons also increases with increasing $Q^2$. One of the most notable findings is that the quarks and anti-quarks only carry about half of the proton’s momentum, and the remainder is contained in the gluons. We should keep in mind that PDF does not provide any information on correlations among the partons.

![Figure 2.1: Probability distribution of momentum fraction of partons inside the proton measured by HERA](image)

(a) Scale of the probe is $Q^2 = 1.9 \text{ GeV}^2$. (b) Scale of the probe is $Q^2 = 10 \text{ GeV}^2$.

2.1 Towards understanding the microscopic structure of the QGP

The phenomena such as scaling violations observed in the initial state structure function of the proton, final state parton fragmentation function, and running of the strong coupling constant have shown that the resolution scale dependence is one of QCD’s fundamental properties. To establish the connection and implications of the scale dependence for high energy jets traversing the QGP, we show a schematic diagram of the scattering of electron off the proton in Fig. 2.2. The left panel shows that the proton’s structure as probed by the electron depends on the spatial resolution or the momentum transfer ($Q^2$) between...
electron and proton. At $Q^2 \sim \Lambda_{\text{QCD}} \approx 200 \text{ MeV}$, the quarks and gluons are subjected to confinement. Due to this, the proton appears to be a cloud of a positively charged object. At an intermediate energy scale, an electron can resolve the short-distance structure of proton, and electron-proton scattering occurs from the constituent valence quarks. Increasing the electron’s energy further, thereby increasing the $Q^2$, the proton appears to be a sea of virtual quarks and gluons. The HERA collaboration at DESY Hamburg [7] has performed a series of $e-p$ DIS experiments and rigorously quantified the structure of proton in terms of parton distribution functions (Fig. 2.1).

Following the DIS analogy, we sketch an analogous process for the case of the hard parton traversing the QGP [see Fig. 2.2(b)]. In the limit of high energy, the hard parton will undergo multiple scatterings in which subsequent scatterings are independent. In Fig. 2.2(b), we illustrate one such scattering event and demonstrate that the QGP will also reveal short-distance structures depending on the resolution scale of the hard parton. The light red oval-shaped blob represents the entire QGP (an extended QCD system), whereas the dark red blob represents the struck portion of the QGP over which the gluon fields are correlated. Qualitatively, lowering the energy of the hard parton would lead to poor resolving power, and the hard parton will see the struck portion of the QGP as an extended fluid. At intermediate energy scales, the hard parton would probe the individual quasi-particles within the struck portion of the QGP. Increasing the hard parton energy further, the struck portion of the QGP would appear to be filled with the sea of virtual quarks and gluons. The primary focus of this thesis is to characterize the QGP at different length scales of the probe. We shall explore the nature of the QGP degree-of-freedom (QGP-DOF), as depicted in Fig. 2.2(b). The momentum exchange between the hard parton and medium parton can range from a value as low as $\Lambda_{\text{QCD}}$ and as high as the scale of the hard parton. In this thesis, we would employ techniques from perturbative QCD, lattice gauge theory, and Monte Carlo based multi-stage energy-loss approach to study the QGP’s multi-scale dynamics.

The study carried out in this thesis would closely follow the philosophy outlined in the
Figure 2.2: (a) Proton as seen by the electron at different resolution scale. Structure of proton is a scale dependent phenomenon. (b) Extending DIS analogy to hard parton going through QGP. Structure of QGP as seen by the hard parton should depend on the scale of the probe.

2015 Long Range Plan for Nuclear Science document [8]. In Fig. 2.3, we show the resolving power achieved by jets produced in ultra-relativistic nucleus-nucleus collisions at RHIC and LHC. The plot also shows the range of the QGP temperature and $p_T$ of the jets created at RHIC and LHC collision energies. The high energy jets generated in the initial hard interaction of the colliding beams provide new microscopes with great potential to explore the inner working of the QGP. These high energy partons in the early stage of propagation will experience the high-temperature QGP and “see” weakly coupled “bare” quarks and gluons in the QGP; this region is highlighted by green color microscope. As the hard parton propagates further, it loses energy via medium-induced gluon emissions and experiences the QGP at lower temperatures. In this region (highlighted by a yellow color microscope), the resolution scale drops, and the scattering is manifested through thermal quasi-particles in the plasma. We also note that the jets produced at RHIC collision energies are an order of
magnitude smaller in energy and hence, probes the longer wavelength and "sees" QGP as a nearly perfect liquid. This corresponds to the region between the orange color microscope and the yellow color microscope.

![Figure 2.3: High energy partons can be used to probe very short distance structure of QGP. This Fig. shows the Long range plan of RHIC and LHC philosophy presented in Ref. [8].](image)

The modification of the leading parton through QGP at different temperatures and length scales shall be encoded in terms of transport coefficients that characterizes the strength of the interaction between the hard parton and QGP. Among existing transport coefficients of jet energy-loss, $\hat{q}$ is a leading coefficient that controls the modifications of the leading parton. The transport coefficient $\hat{q}$ is defined as the average of the squared transverse momentum broadening per unit length for the leading parton through the QGP. The transport coefficient $\hat{q}$ introduces the momentum transverse to the leading parton’s direction by changing its virtuality and, thus, controls the modification of the leading parton through QGP. Given the multi-scale nature of the probe [Fig. 2.2(b)] and a wide plasma temperature range (Fig. 2.3), we shall revisit the energy-loss formalism and attempt to characterize the inner
structure of the QGP in terms of PDF similar to the case of DIS on the proton. This study will demonstrate that there is a non-trivial scale dependence in addition to the known temperature dependence in the transport coefficient $\hat{q}$.

To understand the modification of the leading parton and nature of the QGP at different length scales, we shall study the phenomenon [Fig. 2.2(b)] using three different techniques. In the first approach, we shall focus on a regime in which the hard parton is highly energetic, and the exchanged momenta between the leading parton and QGP are at a perturbative scale. We shall reformulate the transport coefficient $\hat{q}$ using perturbative QCD within the higher-twist energy-loss framework. In the second approach, we shall include the momenta of all scales, both perturbative and non-perturbative, within the framework of lattice QCD. In the third approach, we shall formulate the modification of the leading parton by combining the high-virtuality and low-virtuality phases of the parton energy-loss using the Monte-Carlo approach within the framework of Jet Energy-loss Tomography with a Statistically and Computationally Advanced Program Envelope (JETSCAPE). In this approach, we shall perform hadron-$R_{AA}$ and as well as jet-$R_{AA}$ model-to-data comparisons to set constraints on the mechanism of jet energy-loss. In the next subsections, we briefly discuss three approaches explored in this thesis and present the layout of the thesis.

2.1.1 Constraints on the inner-structure of QGP using perturbative approach

In the first portion of this thesis, we shall focus on the process presented in Fig. 2.2(b) in a regime where the exchanged momenta are at a perturbative scale. We shall consider a realistic case where an energetic and highly-virtual hard parton undergoes transverse momentum broadening due to the multiple scatterings before escaping the plasma. Based on the assumption that the multiple scatterings inside the plasma are incoherent in the high-energy and high-virtuality phase of the parton shower, we introduced a new concept of the Parton Distribution Function (PDF) for the struck portion of the plasma representing an independent scattering center. The leading energy-loss coefficient $\hat{q}$ characterizing the transverse momentum broadening of the hard parton will be reformulated and expressed in terms
of the QGP-PDF [40]. We shall demonstrate that the scale evolution of the QGP-PDF gives rise to a scale dependence in the transport coefficient \( \hat{q}(T, E, \mu^2) \). Moreover, we shall fold this new \( \hat{q}(T, E, \mu^2) \) in the medium-modified fragmentation function within the higher-twist energy-loss formalism.

This analysis would employ (2+1)D viscous hydrodynamical profiles to determine the medium properties. We shall perform a model-to-data comparison of hadron-\( R_{AA} \) at RHIC and LHC energies to extract the scale dependence of \( \hat{q} \), which will elucidate the inner-structure of the QGP in terms of a QGP-PDF. Chapter 3 will serve as a brief theoretical background of the higher-twist energy-loss formalism and medium-modified DGLAP evolution equation. In this chapter, we will also review the work done by the JET collaboration. In Chapter 4, we will present our new work on how to constrain the inner-structure of the QGP in terms of the PDF. We would also demonstrate that the scale dependence in \( \hat{q} \) provides a satisfactory solution of the well known “JET collaboration \( \hat{q} \) puzzle” [discussed in Chapter 3].

2.1.2 Constraints on the temperature dependence of transport coefficient \( \hat{q} \) using lattice gauge theory

In this approach, we shall study the process shown in Fig. 2.2(b) by formulating the interaction between the exchanged gluon and the medium in a non-perturbative environment within the framework of lattice QCD. We shall perform a first-principles calculation in which momenta of all scales are included in \( \hat{q} \). In this calculation, the QGP will be modeled using (2+1)-flavors of quarks, using the highly improved staggered quark action (HISQ) and tree-level Symanzik improved gauge action [41,42]. We shall perform the calculation in a wide range of temperatures, ranging from \( 200 \text{ MeV} \leq T \leq 800 \text{ MeV} \) using the Multiple Instruction & multiple data (MIMD) Lattice Computation (MILC) code package [43,44]. This range is directly relevant to the plasma produced at RHIC and LHC collision energies. It will be demonstrated that this state-of-the-art calculation provides a parameter-free determination of \( \hat{q} \) that has no cusp-like temperature dependence. In chapters 5 and 6 we will discuss this in
great details. In chapter 5, we present a brief review of the essential elements of lattice QCD. In this chapter, we shall discuss the underlying concept in setting up fermions and gauge fields on quenched and unquenched SU(3) lattices. In chapter 6, we will present our lattice formulation of transport coefficient $\hat{q}$. We shall present our estimates of the temperature dependence of $\hat{q}$ for pure gluon plasma and 2+1 flavor quark-gluon plasma cases.

2.1.3 Scale dependence of jets, beyond the transport coefficient $\hat{q}$

In the third portion of the thesis, we shall focus on including the multiple scales and regions involved in the parton energy-loss, as depicted in Fig. 2.3. A complete description of jet modification in QGP must address the role and interplay of the physics at each of these scales and their effect on a leading hadron and as well as on jet observables. In chapter 7, we present such a comprehensive study by performing a model-to-data comparison for leading hadrons and inclusive jets. We shall demonstrate, for the first time, a simultaneous description of the nuclear modification factor for single hadrons and inclusive jets within a unified multi-stage framework which spans multiple centralities and collision energies.

Highlighting one of the major successes of the JETSCAPE event generator [16,45,46], this multi-scale approach includes a high-virtuality radiation dominant generator (MATTER), followed by a scattering dominant (LBT). Each stage transitions to the next phase at a parton-by-parton level, depending on local quantities such as the parton’s energy, virtuality, and the local density. Since jet observables are sensitive to the modification of the soft parton in addition to the hard parton, we incorporated a weakly coupled description of the jet-medium interaction using recoil. Measurements of jet and single hadron $R_{AA}$ set strong constraints on the phase-space available for each stage of the energy-loss.
CHAPTER 3 REVIEW OF THE HIGHER-TWIST ENERGY LOSS

In this chapter, we present a brief theoretical background of the higher-twist energy loss formalism. We shall discuss the notion of factorization in a heavy-ion collision, an important tool to study scattering processes in a high-energy limit. We shall outline salient features of the single-scattering-induced emission within the higher-twist energy loss formalism. Then, discuss the extension to a multiple emission formalism and establish the medium-modified DGLAP evolution equation. We point out that the higher-twist formalism will be the basis for the parton energy loss throughout this thesis. In the end of this chapter, we will review the work done by the JET collaboration.

3.1 Collinear factorization in proton-proton collision

The application of perturbative methods to study scattering processes involving hadronic states in the initial or final state using QCD Lagrangian density differs considerably from studying QED processes. In non-QCD like scattering processes, the fundamental fields appearing in the Lagrangian density are the same as the fields whose quantum number characterizes the initial and final asymptotic states. Whereas in the QCD case, the quanta of the fundamental quark and gluon fields appearing in the QCD Lagrangian density are never observed in the asymptotic states but in the form of composite hadrons. The technical machinery to tackle this issue is referred to as “Factorization” and developed by Collins, Soper, Sterman [47–50]. In this method, one introduces partonic states as intermediate states with quantum numbers of the quark and gluon fields and isolates a section of the scattering process, which can be computed using a perturbative expansion in $\alpha_s$, from the remaining portion of the scattering process which would be non-perturbative.

On applying factorization theorem to ultra-relativistic proton-proton collisions, one can write down the probability to detect a final-state hadron (h) with transverse momentum $p_T$
and rapidity interval \([y, y + dy]\) as

\[
\frac{d^2\sigma_{pp}(p_T, y)}{d^2p_Tdy} = \int dx_a dx_b G_a(x_a, Q^2) \times G_b(x_b, Q^2) \\
\times \frac{d\sigma_{ab\to cX}}{d\hat{t}} \times \frac{D^b_c(z, Q^2, p_c)}{\pi z} + O\left(\frac{\Lambda_{QCD}^2}{Q^2}\right),
\]

where \(G_a(x_a, Q^2)\) and \(G_b(x_b, Q^2)\) are scale dependent parton distribution function (PDF) for incoming protons, respectively. The variable \(x_a(x_b)\) represents the momentum fraction of the incoming partons. The term \(d\sigma_{ab\to cX}/d\hat{t}\) represents the differential cross section to produce a high transverse momentum \((p_{cT})\) parton \(c\) from the hard scattering between the hard parton \(a\) and the hard parton \(b\), where \(\hat{t} = (p_a - p_c)^2\) is a Mandelstam variable. The \(D^b_c(z, Q^2, p_c)\) is called fragmentation functic, and represents the probability for a parton \(c\) to produce a hadron (\(h\)) with momentum fraction \(z\) of the outgoing hard parton. The \(Q^2\) represents the factorization scale (hard scale) up to which the FF \((D^b_c(z, Q^2_0, p_c))\) and PDF \((G_a(x_a, Q^2_0)\) and \(G_b(x_b, Q^2_0))\) should be evolved to from their known form at a lower scale \(Q^2_0\). The last term \(O\left(\frac{\Lambda_{QCD}^2}{Q^2}\right)\) represents higher-order corrections that are suppresed by the powers of the hard scale \(Q^2\) and therefore, are dropped in the calculation.

Note that the primary purpose of the factorization theorem is to factor out the short-distance physics (hard-scale) from the long-distance (soft scale) physics, based on the assumption that there is no interference among them. In Eq. 3.1 only the hard partonic cross section can be computed using pQCD. The non-perturbative quantities PDF or FF can not be calculated explicitly using pQCD, but their scale dependence can be derived by means of renormalization of collinear divergences within the framework of pQCD. Such renormalization introduces a scale dependence in PDF and FF, and give rise the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equation \[51\text{–}\text{54}\],

\[
\text{PDF : } \frac{\partial G_i(x, \mu^2)}{\partial \ln \mu^2} = \frac{\alpha_s(\mu^2)}{2\pi} \sum_j \int_x^1 \frac{dy}{y} P_{i\to j} \left(\frac{x}{y}\right) G_j(y, \mu^2)
\]

(3.2)
\[
\text{FF :} \quad \frac{\partial D^h_i(z, \mu^2)}{\partial \ln \mu^2} = \frac{\alpha_s(\mu^2)}{\pi} \sum_j \int_{z}^{1} \frac{dy}{y} P^{i\rightarrow j}_+(y, \alpha_s) D_j^h \left( \frac{z}{y}, \mu^2 \right). \quad (3.3)
\]

There is a striking similarity between DGLAP equations for PDF and FF. At LO, the splitting functions \(P^{i\rightarrow j}_+\) are the same and only differ at NLO and have been computed in Ref. [55, 58]. The subscript \(+\) on the splitting function indicates that the virtual corrections are included. These PDF’s and FF’s are universal functions, and are determined by performing a model-to-data comparison of differential cross section observables at one value of the scale.

### 3.2 Collinear factorization in heavy-ion collision

In ultra-relativistic nucleus-nucleus collisions, calculation of high-\(p_T\) leading hadron suppression provides an important tool to investigate the properties of the QGP medium. Such calculations require the factorization of the initial state effects and final state effects from hard parton-parton scattering. This factorization is generally assumed to hold for the case of a nucleus-nucleus collision with some caveats. In this factorized approach, one can write the total probability to detect a final state hadron \((h)\) with transverse momentum \(p_T\) and rapidity interval \([y, y + dy]\) as

\[
\frac{d^2\sigma^{AA}(p_T, y)}{d^2p_T dy} \bigg|_{b_{\text{min}}}^{b_{\text{max}}} = K \int_{b_{\text{min}}}^{b_{\text{max}}} d^2b \int d^2r_A(r) t_B(r - b) \times \int dx_a dx_b G_a^{A}(x_a, Q^2) \times G_b^{B}(x_b, Q^2) \\
	imes \frac{d\sigma_{ab\rightarrow cX}}{dt} \times \frac{\tilde{D}^h_c(z, Q^2, \zeta_L(r, \theta_j), p_c)}{\pi z} + O \left( \frac{\Lambda_{\text{QCD}}^2}{Q^2} \right),
\quad (3.4)
\]

where \(G_a^{A}(x_a, Q^2)\) and \(G_b^{B}(x_b, Q^2)\) are scale-dependent initial state nuclear structure function for incoming nucleus \(A\) and \(B\) taking into account the effects from nuclear shadowing, respectively. The variable \(x_a(x_b)\) represents the momentum fraction of the incoming partons. The \(Q^2\) represents the hard scale up to which initial state structure function \(G_a^{A}(x_a, Q^2)\) and \(G_b^{B}(x_b, Q^2)\) should be evolved to using their known form at a lower scale \(Q^2_{0}\). The term \(K\) is
a multiplicative factor to account for higher-order corrections. The $t_{A/B}(\vec{r} \pm \vec{b}/2)$ represents the nuclear thickness function given as $t_A(\vec{r} + \vec{b}/2) = \int dz \rho(\vec{r} + \vec{b}/2, z)$, where $\rho(\vec{r}, z)$ is the nucleon density inside a nucleus. The term $d\sigma_{ab\to cX}/d\hat{t}$ represents the differential cross section to produce a high transverse momentum ($p_{cT}$) parton $c$ from the hard scattering of the hard parton $a$ with the hard parton $b$, where $\hat{t} = (p_a - p_c)^2$ is a Mandelstam variable. The function $\tilde{D}^b_c(z, Q^2, \zeta_L(\vec{r}, \theta_j), p_c)$ represents the medium modified fragmentation function [see Eq. (3.15)], where $z = p_T/p_{cT}$ and $\zeta_L(\vec{r}, \theta_j)$ is the distance traveled by the leading parton $c$ produced at $\vec{r}$ and propagating at an angle $\theta_j$ with respect to reaction plane angle. The $\vec{b}$ and $\vec{r}$ are two-dimensional vectors transverse to the beam direction.

Note, initial state distributions are assumed to be obtained from standard PDFs, with minor nuclear modifications such as shadowing, and the hard partonic cross section can be reasonably factorized from the evolving medium. While this is not obvious for the partons in the final state and the fragmentation function, but for the case of very high energy partons (produced after the hard scattering), can it be reasonably argued that a considerable portion of the jet will escape the medium, with the fragmentation of the leading hadron being unaffected by the medium. In this case, one may use a vacuum fragmentation function to describe the hadronization of the leading hadron.

Even in this case, the propagation of the jet through the medium will affect the partonic structure of the jet. Its modification in the medium is caused by scattering, drag, and medium induced radiation from the hard partons in the shower. These modifications are controlled by non-perturbative transport coefficients, which are assumed to be factorized from the propagation of the hard partons. While there are several such coefficients which encode the effect of the non-perturbative medium on the shower partons, the leading transport coefficients are the transverse momentum diffusion coefficient $\hat{q}$, and the longitudinal drag coefficient $\hat{e}$. The transport coefficients such as $\hat{q}$ are universal functions and set using one or two data points from leading hadron suppression in heavy-ion collisions. In this thesis, we will focus exclusively on $\hat{q}$. In subsequent section, we will discuss how the transport
coefficient $\hat{q}$ arises in the calculation of the parton energy-loss and discuss how to set up a medium-modified DGLAP equation within the framework of higher-twist formalism.

3.3 Higher-Twist formalism

One of the challenging problems in explaining the high-$p_T$ hadron observables in a heavy-ion collision is understanding jet modification due to interactions with the QGP. In this section, we outline salient assumptions made in such a calculation and discuss specifically how the transport coefficient $\hat{q}$ (quenching parameter) is factorized in the higher-twist based parton energy loss formalism. To do this, one considers an analogous process of deep-inelastic scattering on a large nucleus ($A \gg 1$) at large photon virtuality ($Q^2 \gg \Lambda_{QCD}$) and focus in the limit where a hard quark is produced after the scattering.

In this limit, we can factorize the propagation of the quark in the extended nuclear medium (large nucleus) from the production process, obtaining equations for the scattering-induced single gluon emission spectrum or the transverse momentum distribution of the produced quark. We have shown a scattering-induced single gluon emission diagram in Fig. 3.1(a). In general, the twist of a Feynman diagram containing the non-perturbative operators is given by the difference of the total dimension of the operator product and total spin (maximum) of the quark and gluon field operators involved in the operator product.

The leading twist diagram for photon-nucleus scattering does not include the effects of the nuclear medium and has a twist number as 2. The next-leading twist diagram includes medium scattering (shown in Fig. 3.1(a)) and has a twist number as 4. The analytical calculations of such processes is carried out in the Breit frame where the virtual photon $\gamma$ and the nucleus have momentum four-vectors $q = [-Q^2/2q^- , q^- , 0 , 0]$ and $P \equiv [P^+ , 0 , 0 , 0] = A[p^+ , 0 , 0 , 0]$, respectively, where $A$ is the mass number and $q^-$ is the large light-cone momentum of the hard quark. We choose the nucleus [grey shaded square box in Fig. 3.1(a)] to be traveling in the positive $z$-direction with large light-cone momentum $P^+ = Ap^+$ and the photon in the negative $z$-direction. In this frame, the Bjorken variable is given as $x_B = Q^2/2p^+q^-$. We define the momentum of a struck quark or gluon
in any of the nucleons in terms of momentum fraction \(x\) as \(p_{q,g} \simeq xp\) (where \(0 < x < 1\)), where \(p\) is four-momentum of the nucleon. In this picture, each nucleon is time dilated to an almost static state with an arbitrary number of near on-shell quarks and gluons, which are described by the PDF of the nucleon (in this study, we will ignore nuclear effects on the nucleon PDF).

Now, we consider a scenario where a hard quark propagates through the nucleus. It undergoes multiple scatterings off the gluon field of the nucleus and radiates gluons. We consider this process in the limit where the hard parton carries high energy and high virtuality. In this limit, the hard parton propagation would be radiation dominant with a few scatterings. It would be a reasonable assumption to assert that the scatterings would be independent and take place on separate nucleons, i.e. double scatterings on a single nucleon would be rare. Thus, the exchanged gluon coming off a nucleon will not be correlated to other nucleons in the nucleus. While traversing the nucleus, scattering also induces radiation, in addition to the vacuum radiation emanating from the hard quark. The Fig. 3.1(b) shows different ways in which the hard parton’s energy and virtuality gets modified while traversing a nucleon. For the case where only the radiated gluon scatters with the nucleon, the differential yield of induced gluons in bins of light-cone momentum fraction \(y\) and transverse momentum \(\vec{l}_\perp\) from a single scattering can be expressed as \(59\)–\(61\),

\[
dN_g \frac{dy dl^2_\perp}{dy} = \frac{\alpha_s}{2\pi^2} P(y) \int \frac{d\zeta^- d\delta \zeta^- d^2 k_\perp d^2 \zeta_\perp}{(2\pi)^2} \left[ \frac{2 - 2 \cos \left\{ \frac{(l_\perp - k_\perp)^2 \zeta^-}{2q \gamma (1-y)} \right\}}{(l_\perp - k_\perp)^4} \right] e^{-i \frac{k^2_\perp}{2q} \delta \zeta^- + i k_\perp \cdot \zeta_\perp} \times \left\langle p_B \big| A^{a+}(\zeta^- + \delta \zeta^- , \zeta_\perp) A^{a+\dagger}(\zeta^- , 0_\perp) \big| p_B \right\rangle.
\]

(3.5)

where, \(l_\perp\) and \(y\) are the transverse momentum and longitudinal momentum fraction of the radiated gluon, respectively. \(P(y)\) is the regular AP splitting function.

The scattering takes place at the location \((\zeta^- , 0_\perp)\) in the amplitude and at the shifted location \((\zeta^- + \delta \zeta^- , \zeta_\perp)\) in the complex conjugate, where \(A^{a+}\) represents the dominant component of the gluon field at these locations \((A^{a-} = 0\) gauge) in the nucleon state \(|p_B\rangle\).
Requiring that the final nuclear state be identical in both amplitude and complex conjugate, the \( \delta\zeta^- \) and \( \zeta^- \) integrals are limited by the size of a nucleon, i.e., the same nucleon that is struck in the amplitude is also struck in the complex conjugate. The \( \zeta^- \) integral is limited by the formation time of the radiation \( \tau^- \) or the light-cone length \( L^- \) that has to be traversed in the nucleus by the parton. The scattering exchanges a transverse momentum \( \vec{k}_\perp \) between the radiated gluon and the medium, along with plus-component of the momentum \( k^+ = k^2_\perp/(2q^-) \), and negative-component of the momentum \( k^- = k^2_\perp/(2p^+q^-) \).

Although not made clear in prior publications, there is a tension between the integrand in the first and second lines of Eq. 3.5 regarding the dominant range of the \( k_\perp \) integration. Although explicitly demonstrated in the subsequent sections, it is immediately clear that the expectation of the operator product in the third line of Eq. 3.5 is enhanced for separations \( \zeta_\perp \approx 1/p_{B\perp} \approx 1/\Lambda_{QCD} \). Thus, the matrix element prefers \( k_\perp \approx \Lambda_{QCD} \). However, the integrand in the first line of Eq. 3.5 prefers \( k_\perp \approx l_\perp \), the transverse momentum of the radiated gluon. This is consistent with the idea of coherence first expounded in Refs. [62–64].

To clearly illustrate this, we briefly make the approximation that, in a large nucleus, one can assume longitudinal translation invariance of the matrix element, i.e., on average, all nucleons are similar and, thus,

\[
\left\langle p_B \left| A^{a+}(\zeta^- + \delta\zeta^-, \vec{\zeta}_\perp)A^{a+}_\alpha(\zeta^-) \right| p_B \right\rangle \approx \left\langle p_A \left| A^{a+}(\delta\zeta^-, \vec{\zeta}_\perp)A^{a+}_\alpha(0) \right| p_A \right\rangle. \tag{3.6}
\]

In the above expression, nucleon \( A \) is at the origin \( \vec{\zeta} = 0 \), and nucleon \( B \) is at \( (\zeta^-, 0) \).

In this approximation, we can factorize the location integrals in the first and second lines of Eq. 3.5 obtaining

\[
\frac{dN_g}{dyd\vec{k}_\perp^2} = \frac{\alpha_s}{2\pi^2} P(y) \int \frac{d^2k_\perp}{(2\pi)^2} \int_0^{\tau^-} d\zeta^- 2 - 2 \cos \left\{ \frac{(l_\perp - k_\perp)^2\zeta^-}{2q^-y(1-y)} \right\} \times \int d\delta\zeta^- d^2\zeta_\perp e^{-\frac{i\delta\zeta^- + i\vec{k}_\perp \cdot \vec{\zeta}_\perp}{4q^-}} \left\langle p_B \left| A^{a+}(\delta\zeta^-, \vec{\zeta}_\perp)A^{a+}_\alpha(0) \right| p_B \right\rangle. \tag{3.7}
\]
Figure 3.1: Basic diagrams in higher-twist energy-loss formalism. (a) A typical higher-twist diagram contributing in the modification of the fragmentation function. (b) Diagrams display different ways in which the hard parton’s energy and virtuality could get modified in the presence of the nuclear medium (red oval shaped blob). The blue star indicate that the parton line is more virtual than the remaining parton lines and the label v.c. signifies virtual corrections.

We define the integral in the second line of the Eq. 3.7 as

\[ H(k_\perp, l_\perp, q^-, y) = \tau^- \int_0^1 d\zeta^- \frac{2 - 2 \cos \left\{ \frac{(l_\perp - k_\perp)^2 \zeta^-}{2q^- y (1-y)} \right\}}{(l_\perp - k_\perp)^4}, \] (3.8)

where the formation time \( \tau^- = 2q^-/\mu^2 \) and \( \mu^2 \approx l_\perp^2 \). This function (normalized) is plotted in Fig. 3.2 as a function of \( k_\perp,x \) for two different values of \( l_\perp,x = 5, 50 \text{ GeV} \). We choose the projection along \( k_\perp,y = l_\perp,y = 0, q^- = 50 \text{ GeV}, \) and \( y = 0.5 \).

As one immediately notes, increasing \( l_\perp \), which in transverse space corresponds to making the quark-gluon dipole smaller, selects \( k_\perp \) exchanges that are of the same order as \( l_\perp \), i.e., wavelengths that can resolve the quark-gluon dipole as separate partons. To completely uncouple the terms in the terms in the second line with those in the third and fourth line of Eq. 3.7 a Taylor expansion in \( \frac{k_\perp^2}{l_\perp^2} \) (odd powers vanish due to cylindrical symmetry) is carried out. Using by parts integration, the product \( \int d^2\zeta_\perp i \vec{k}_\perp \exp[i\vec{k}_\perp \cdot \vec{\zeta}_\perp] A^{a+}(\vec{\zeta}_\perp) \) can be converted to \( \int d^2\zeta_\perp \exp[i\vec{k}_\perp \cdot \vec{\zeta}_\perp] \partial_\perp A^{a+}(\zeta_\perp) \approx \int d^2\zeta_\perp \exp[i\vec{k}_\perp \cdot \vec{\zeta}_\perp] F_\perp^{a+}(\zeta_\perp) \), where \( F_\perp^{a+} \) is the gluon chromo-magnetic field transverse to the direction of propagation of the hard parton.

The first non-vanishing contribution, from the term \( \frac{k_\perp^2}{l_\perp^2} \), is contained within the transport
The transport coefficient $\hat{q}$ is the leading property of a strongly interacting medium that effects jet propagation. It introduces momentum transverse to a jet parton’s direction, changing its virtuality and thus controls the modification of hard jets in a dense extended medium. It should be pointed out that while coherence effects (2nd line of Eq. 3.7 above),...
require a $k_\perp \sim l_\perp$ for energy loss to take place on a virtual parton, momentum fluctuations where $k_\perp \gg \Lambda_{\text{QCD}}$, are suppressed in a nucleon. As a result, $\hat{q}\tau^- \ll l_\perp^2$. Extending this argument further, it will be assumed that higher power corrections e.g., $k_\perp^4/l_\perp^4$, which yield terms such as

$$J = \frac{\langle p_B | \partial^\perp F^{a+\alpha}(\zeta^- + \delta\zeta^-, \vec{\zeta}_\perp) \partial_\perp F^{a+\alpha}(\zeta^-) | p_B \rangle}{l_\perp^4},$$

(3.11)

are suppressed compared to the $\hat{q}\tau^- / l_\perp^2$, and are ignored in the remainder of this paper. The reader will note that this statement depends on assumptions regarding the distribution of momentum originating from the nucleon state.

In chapter 4 Sect. 4.4, we will present a phenomenological model which obeys this approximation. Given these, we obtain the medium induced spectrum of gluons radiated from a single scattering in the medium as

$$\frac{dN_g}{dyd^2l_\perp} = \frac{\alpha_s P(y)}{2\pi^2} \int_0^{\tau^-} d\zeta^- \hat{q}(\zeta^-) \frac{2 - 2 \cos \left\{ \frac{(l_\perp)^2 \zeta^-}{2q^-y(1-y)} \right\}}{(l_\perp)^4}.$$  

(3.12)

In the subsequent section, we use the above formula to compose a multiple emission formalism to compute the yield of hadrons fragmenting from the hard parton.

3.4 Multiple emission and medium-modified DGLAP equation

In nuclear collisions at RHIC and LHC energies, the hard partons generated from the initial state hard scattering start out with a virtuality that is much higher than any medium scale. In this stage, medium modification is power suppressed and is a perturbative correction to the virtuality ordered vacuum-like emissions from the hard parton. In this chapter, it will be assumed that partons remain in this state as they exit the large nucleus (dense medium), and then fragment in the vacuum to produce hadrons. This picture is obviously not accurate for most of the hadrons that emanate from this process, and many will be produced within or will be affected by the nuclear medium. However, this picture is appropriate for the highest energy hadrons which are produced in the fragmentation of the highest energy parton, which is expected to exit the nuclear medium prior to fragmentation.
In the case of the vacuum, the yield of hadrons carrying a momentum fraction \( z \) of the original parton from the fragmentation of a single parton with virtuality \( \mu_0^2 \), is obtained using the fragmentation function \( D(z, \mu_0^2) \). The change of the yield due to multiple emissions from a parton with different virtuality \( \mu^2 \) is obtained as,

\[
D(z, \mu^2) = D(z, \mu_0^2) + \int \frac{d\mu_1^2}{\mu_0^2} \int \frac{1}{z} \frac{dy}{y} P_+(y) D \left( \frac{z}{y}, \frac{\mu^2}{\mu_0^2} \right) + \ldots, \tag{3.13}
\]

where the \( \ldots \) represent 2 and the higher number of emissions. The subscript + on the splitting function indicates that we have subtracted the virtual correction which contains the product of the leading amplitude, and the next-to-leading order complex conjugate for no emission (and vice-versa). This virtual correction removes the infra-red divergence from soft gluon emission in the splitting function.

In Fig. 3.3, we show virtuality ordered emission diagrams that contributes to the scale dependence of vacuum fragmentation function. Contributions from multiple emissions can be resummed by solving the DGLAP evolution equation,

\[
\frac{\partial D^h_i(z, \mu^2)}{\partial \log \mu^2} = \sum_j \frac{\alpha_s}{2\pi} \int dy P_i \to j(y) D^h_j \left( \frac{z}{y}, \mu^2 \right). \tag{3.14}
\]

In order to add the contribution from medium induced emission, we simply convert from transverse momentum to virtuality \( l_\perp^2 = \mu_1^2 y (1 - y) \) in Eq. 3.12 and integrate \( \mu_1^2 \) from \( \mu_0^2 \) to \( \mu^2 \). The ensuing term can be added to the kernel of the DGLAP equation above to obtain the medium modified DGLAP evolution equation. Given the form of Eq. 3.12 one necessarily obtains a medium modified fragmentation function \( \tilde{D}(z, \mu^2, \zeta^-) \| q^- \), which additionally depends on the light-cone momentum \( q^- \) of the hard parton, and on the location \( \zeta^- \), where the parton is produced in the medium (\( z \) is the momentum fraction carried by the hadron with respect to the parent parton, and \( \mu^2 \) is the scale of the function or the virtuality of the parton).
The medium-induced single-emission kernel is represented by the grey blob (zoomed as square box) in Fig. 3.3(b) which is repeated in the limit that the successive emissions are virtuality ordered. In figure 3.3(b), the red shaded blob represents the medium, whereas the blue star in square box indicated that the parton line is more virtual than the remaining parton lines in the diagram. Including series of such diagrams with multiple scattering with one emission per scattering give rise to the following in-medium-DGLAP evolution equation [59,65],

\[
\frac{\partial \tilde{D}^h_i (z, \mu^2, \zeta^-)}{\partial \log \mu^2} \bigg|_{q^-} = \sum_j \frac{\alpha_s(\mu^2)}{2\pi} \int_z^1 \frac{dy}{y} \left\{ P^{i\to j}(y) \tilde{D}^h_j \left( \frac{z}{y}, \mu^2, \zeta^- \right) \bigg|_{yq^-} \right. \\
+ \left. \left[ \left( \frac{P^{i\to j}(y)}{y(1-y)} \right) + \tilde{D}^h_j \left( \frac{z}{y}, \mu^2, \zeta^- + \tau^- \right) \bigg|_{yq^-} \right] \right. \\
\times \left. \int_{\zeta^-}^{\zeta^- + \tau^-} d\zeta^- \frac{\hat{q}(\zeta^-)}{\mu^2} \left\{ 2 - 2 \cos \left( \frac{\zeta^-}{\tau^-} \right) \right\} \right\}.
\]
where $P_{i \rightarrow j}(y)$ and $\tilde{D}_{i}^{h}(\frac{\xi}{y}, \mu^2)$ represents the Altareli-Parisi splitting function and medium-modified fragmentation function, respectively. The factor within the square bracket in equation (3.15) comes from the interference between different scattering diagrams. The light-cone coordinate $\xi_{i}$ and $\xi$ corresponds to the origin of the jet-like parton, and the space-time location of parton-medium scattering vertex. The coordinate $\xi_{f}$ represents the location at which the parton exits the medium.

The equation with the term $P_{i \rightarrow j}^{i}(y) \tilde{D}_{i}^{h}(\frac{\xi}{y}, \mu^2, \zeta_{-i})|_{yq^{-}}$ alone on the first line of Eq. 3.15, is identical to the evolution equation of the vacuum fragmentation function, except that the functions now also depend on the origin of the hard parton. The quantity within the square bracket represents the medium modified portions, which mixes functions at location $\zeta_{-i}$ with partons formed ahead in the medium by a formation time $\tau_{-} = 2q^{-}/\mu^2$.

Also, we note that the parent parton’s energy $q^{-}$ (or $yq^{-}$) is separate from the other variables in the fragmentation function. This is because the rescaling of the energy on the right-hand side of the DGLAP equation takes place in the case of Eq. 3.14 as well, but is usually suppressed as vacuum fragmentation functions are invariant under boosts in the parton’s direction. In the presence of a medium, the fragmentation functions are no longer boost invariant. However, parametrically, this is not a new dependence such as the position dependence.

The position-dependent quantity $\hat{q}(\xi)$ in equation 3.15 represents the average transverse momentum ($\vec{k}_{\perp}$) broadening per unit length ($L$) of the medium. The transport coefficient $\hat{q}$ is the leading property of a strongly interacting medium that effects jet propagation. It introduces momentum transverse to a jet parton’s direction, changing its virtuality and thus controls the modification of hard jets in a dense extended medium. Notice, in Eq. 3.15 the $\hat{q}(\xi)$ depends only on the location $\xi$, but in the next chapter, we will demonstrate that $\hat{q} \equiv \hat{q}(\xi, q^{-}, \mu^2)$ not only depends on the location $\xi$, but also on the hard parton’s energy $q^{-}$, and the scale $\mu^2$. This would be one of the goals of the subsequent chapter.
3.5 Single-hadron suppression and JET collaboration $\hat{q}$ puzzle

The ultra-relativistic nucleus-nucleus collisions performed at RHIC and LHC in the past decades have produced a plethora of experimental data that confirmed the phenomenon of jet quenching in QGP. The jet quenching patterns have been seen in the measurements of high-$p_T$ inclusive hadron spectra \cite{66-68}, $\gamma$-hadron correlations \cite{69,70}, dihadron correlations \cite{6}, reconstructed inclusive jets \cite{71,72}, dijet \cite{73,74} and $\gamma$-jet asymmetry \cite{75}. These observables have been studied by a variety of pQCD based parton energy loss models. Although most of these models could describe the jet quenching pattern observed at RHIC and LHC by adjusting the free parameters in their respective models, the underlying assumptions across various models are quite different. In addition to that, the simultaneous description of jet quenching observables at RHIC and LHC collision energies remains a challenging task.

In this section, we discuss the first rigorous phenomenological study of the suppression of the leading hadrons carried out by the JET collaboration \cite{9}. For five different parton energy-loss models, systematic model-to-data comparisons were performed by constraining the nuclear modification factor hadron-$R_{AA}$ at RHIC and LHC energies. The nuclear modification factor $R_{AA}$ measures the suppression of the leading hadron and is expressed as the ratio of the differential yield of hadrons $d^2N_{AA}(b_{min}, b_{max})$ in bins of $p_T$, rapidity ($y$), and centrality (codified by a range of impact parameters $b_{min}$ to $b_{max}$) in a nucleus-nucleus collision, to the differential yield of hadrons in a proton-proton (pp) collision, scaled by $\langle N_{bin}(b_{min}, b_{max}) \rangle$, the average number of expected nucleon-nucleon collisions in the same centrality bin. The calculations performed were for the most central (0-5\%) events at the RHIC ($\sqrt{s} = 200$ GeV per nucleon) and LHC ($\sqrt{s} = 2.76$TeV per nucleon) collision energies. These calculations were run on identical (2 + 1)D viscous hydrodynamical profiles from Ref. \cite{76-78}.

The five different approaches to the parton energy loss were GLV-CUJET, HT-M, HT-BW, MARTINI, and McGill-AMY \cite{9}. To model the parton energy loss, CUJET implements a potential model for multiple scattering with the medium in which the strong coupling
constant $\alpha_s$, Debye mass, and density of scattering centers are free parameters determined from fits to hadron-$R_{AA}$. The parton energy-loss in higher-twist approaches (HT-BW and HT-M) encoded the medium effects using the transport coefficient $\hat{q}$. The hard-thermal-loops (HTL) based parton-energy loss models (MARTINI and McGill-AMY) have a strong coupling constant as an adjustable parameter. To compare these differing formalism on equal-footing, each model computed transport coefficient $\hat{q}$ based on the extracted parameters. In higher-twist and HTL based parton energy-loss approaches, $\hat{q}$ was employed as

\begin{align}
\text{HT-M: } \hat{q} &= \hat{q}_0 \frac{s}{s_0} \\
\text{HT-BW: } \hat{q} &= \hat{q}_0 \frac{\rho}{\rho_0} \\
\text{MARTINI and McGill-AMY: } \hat{q} &= \alpha_s C_a m_D^2 T \log \left( 1 + \frac{6E}{T} \right) 
\end{align}

where, $\hat{q}_0$ and $\alpha_s$ are free parameters, $s$ is the average local entropy density, $s_0$ is the maximum entropy density achieved in most central collisions at $\tau_0 = 0.6$ fm/c, $\rho$ is the average local density of the medium, $\rho_0$ is a constant, $C_a$ is Casimir factor, $m_D^2$ is the Debye thermal mass, $T$ is the average local temperature of the medium and $E$ is the energy of the parton in the rest-frame of medium.

The above $\hat{q}$ parametrization has one free parameter that is estimated through fitting the experimental data to the full model calculation. In Fig. 3.4(a), we show inclusive hadron-$R_{AA}$ at RHIC and LHC collision energies using HT-M energy loss approach for different values the free parameter $\hat{q}_0$. The best fit for case of RHIC data yield the $\hat{q}_0 = 2.0$ GeV$/c^2$ fm, whereas for LHC data yields $\hat{q}_0 = 2.9$ GeV$/c^2$ fm. The $\hat{q}$ extracted are for the gluon jets. To obtain the $\hat{q}_0$ for the case of quark one needs to multiply the color factor of $C_F/C_A = 4/9$, where $C_F = (N_c^2 - 1)/(2N_c)$ and $C_A = N_c$. This leads to $\hat{q}$ for quark jets as $\hat{q} = 0.89$ GeV$/c^2$ fm in most central Au+Au collisions (RHIC) and $\hat{q} = 1.29$ GeV$/c^2$ fm in most central
Pb+Pb collisions (LHC) during the initial time $\tau_0 = 0.6$ fm/c. In these calculations hydro profiles were obtained with MC-KLN initial conditions in which the initial temperature ($\tau_0 = 0.6$ fm/c) is $T_0 = 346$ MeV, at the center of the most central $Au + Au$ collisions at RHIC ($\sqrt{s} = 200$ GeV/n) and $T_0 = 447$ MeV in $Pb + Pb$ collisions at LHC ($\sqrt{s} = 2.76$ TeV/n). Thus, the extracted value of the dimensionless parameter $\hat{q}/T^3 \approx 4.2$ at $T = 346$ MeV (RHIC 0-5% centrality), whereas $\hat{q}/T^3 \approx 2.8$ at $T = 447$ MeV (LHC 0-5% centrality). The enhancement of $\hat{q}/T^3$ at lower temperature is in contradiction to the fact that $s/T^3$ diminishes as temperature is decreased. This implies that the parametrization of $\hat{q}$ solely based on local entropy density leads to a puzzle.

In Fig.3.4, we present fits to hadron-$R_{AA}$ at RHIC and LHC collision energies using McGill-AMY model of parton energy loss. For this case, $\hat{q}$ is given by Eq. 3.18 where $\alpha_s$ is the fit parameter. The best fit to the experimental data is shown using the solid thick line in the middle; this gives the extracted value of $\alpha_s = 0.27$ at RHIC and $\alpha_s = 0.24$ at LHC independent of the temperature of the plasma. Here as well, we observe a readjustment of the free parameter is required to describe the experimental data at RHIC and LHC simultaneously. A similar model-to-comparisons were done using HT-BW, MARTINI, and GLV-CUJET energy loss model [9].

The striking outcome of this study was the demonstration that these five energy-loss formalisms although differ considerably in terms of the underlying physics assumptions exhibit a common property: The extracted value of the dimensionless free parameter $Q$ (interaction strength), defined as,

$$\hat{q}(T) = Q \ T^3,$$

from fits to leading hadron $R_{AA}$ was higher at the RHIC collision energy compared to that at the LHC collision energy (at the same temperature). Naively, one would expect $\hat{q}$ to be a universal function of physical quantities, such as the temperature of the plasma, and the interaction strength to be either independent or have a logarithmic dependence on the temperature and energy of the jet as would be indicated via a calculation using hard thermal.
loop effective theory. Instead, the calculations show (Fig. 3.5) that the interaction strength is \( \approx 2 \) times larger for a QGP produced in RHIC collisions compared to a QGP produced in LHC collisions (at the same temperature). This after taking into account the higher temperature range at the LHC, suggests that \( \hat{q} \) is sensitive to other properties that change with the center-of-mass energy of the collision. This odd property is referred to as the JET Collaboration \( \hat{q} \) puzzle (Fig. 3.5).

So far, fewer attempts to explore the possible dependence on the interaction strength
Figure 3.5: First systematic extraction of the temperature dependence of $\hat{q}$ by JET collaboration [9].

$Q$ been made, e.g., in Refs. [10, 79]. The work of the authors of Ref. [79], based on the possibility of magnetic monopoles in the plasma, suggests that the interaction strength $Q$ has a nontrivial (upward cusplike) temperature dependence in the region around $T_c$ (based on the quasi-particle relation derived in Ref. [80]). This implies that experiments at the RHIC are more sensitive to this rise in $Q(T)$ near $T_c$ due to lower initial temperatures at the RHIC, compared to the LHC. As a result, the effective $Q$ extracted in comparison with data tends to be higher at the RHIC than at the LHC.

However, studies performed using quenching weights [81] within the Armesto-Salgado-Wiedemann (ASW) energy loss formalism in past years by the authors of Ref. [10] are in clear contradiction with such a prediction. In this calculation, the quenching parameter $\hat{q}$ is given as:

$$\text{ASW : } \hat{q} = 2K\epsilon^{3/4},$$  \hspace{1cm} (3.20)
where $\epsilon$ is the average local energy density of the medium and $K$ is the free model parameter that controls the quenching. We show $K$ factor extracted from fits to hadron-$R_{AA}$ at RHIC collision energies and LHC collision energies for different impact parameters of the collision. We observe that the extracted $K$ factor at RHIC is roughly $K \approx 2.1\text{-}3.0$, where it is roughly $K \approx 1.0$ at LHC. This means the $K$ factor is $\approx 2\text{-}3$ times larger at RHIC collision energies compared to LHC. Moreover, this formalism reveals that the interaction strength $Q$ is sensitive to the center-of-mass energy of nucleus-nucleus collision rather than the local temperature of the QGP or the centrality of colliding nuclei.

Figure 3.6: The $K$ factor determined from fits to single-hadron $R_{AA}$ at RHIC and LHC collision energies using ASW energy-loss formalism. In this calculation $\hat{q} = 2K\epsilon^{3/4}$, where $\epsilon$ is the local energy density of the QGP and $K$ is universal free parameter that controls the quenching [10].

Note that the initial temperature achieved in a heavy-ion collision (at thermalization) not only depends on the center-of-mass energy of nucleus-nucleus collisions, but also on its centrality. The effect of the cusp at $T_c$ as proposed in Ref. [79] should be much stronger in peripheral collisions compared to most central collisions, leading to noticeably larger suppression than expected based on a monotonic scaling relation between $\hat{q}$ and $T$. Therefore, such cusp-like behaviour in $\hat{q}$ will be in-consistent with the observations made within the
ASW formalism as reported in Ref. [10].

One of the goals of this thesis is to further develop the formalism to study the transport coefficient $\hat{q}$ and demonstrate that at both the RHIC and the LHC, both the centrality dependence of the $R_{AA}$ and azimuthal anisotropy ($v_2$) of leading hadrons can be well described using a $Q$, that has no such cusplike behavior near $T_c$. In the next chapter, we formulate the transport coefficient $\hat{q}$ that depends not only on the local temperature $T$ (local entropy density), but also the energy of the leading parton and the scale at which the leading parton probes the medium. With this, we successfully demonstrate the reduction of $Q$ at the LHC compared to the RHIC is caused mainly due to the scale evolution of $\hat{q}$. Our results have been published in Refs. [40,82,83].
CHAPTER 4 PARTON DISTRIBUTION FUNCTION FOR QGP, AND THE JET COLLABORATION PUZZLE

The goal of this chapter is to characterize the QGP at different length scales of the probe. In this chapter, we present a scale-dependent formalism of the transport coefficient $\hat{q}$, which allows us to explore the nature of the QGP degree-of-freedom (QGP-DOF) as depicted in Fig. 2.2(b). We shall perform a model-to-data comparison of hadron-$R_{AA}$ at RHIC and LHC energies to extract the distribution of quasi-particles inside the QGP at a reference scale $\mu^2 = 1 \text{ GeV}^2$. It will also be demonstrated that the scale-dependence of QGP-PDF provides a satisfactory solution to the JET collaboration $\hat{q}$ puzzle.

4.1 Basic assumptions

Studies done in past decades related to hadronic scattering processes have shown that the resolution scale is one of the fundamental quantities that drives various QCD phenomena such as scaling violations observed in the initial state structure function of the proton (Fig. 2.1), final state parton fragmentation and running of the strong coupling constant. Following the DIS analogy, we sketch an analogous process for the case of the hard parton traversing the QGP. In the limit of high energy, the hard parton will undergo multiple scatterings in which subsequent scatterings are independent of each other. In Fig. 2.2(b), we illustrate one such scattering event and demonstrate that the QGP will also possess short-distance structures depending on the resolution scale of the hard parton.

The light red oval-shaped blob [Fig. 2.2(b)] represents the entire QGP (an extended QCD system), whereas the dark red blob represents the struck portion of the QGP over which the gluon fields are correlated. Qualitatively, lowering the energy of the hard parton would lead to poor resolving power, and the hard parton will see the struck portion of the QGP as an extended fluid. At intermediate energy scales, the hard parton would probe the individual quasi-particles within the struck portion of the QGP. Increasing the hard parton energy further, the struck portion of the QGP would appear to be filled with the sea of virtual quarks and gluons.
To understand the evolution of the microscopic structure of the QGP, we consider a realistic case where an energetic hard parton produced from the initial state hard scattering undergoes transverse momentum broadening due to scattering with the plasma. We assume that the hard parton carries high energy and high virtuality. In this regime, the parton shower is radiation dominant with a few scatterings in the plasma. Moreover, in this case, the multiple scatterings will be considered independent of each other. We illustrate the setup in Fig. 4.1, where the black gluon lines are radiation off the hard quark and the orange gluon lines are transverse gluon exchanged with the plasma. The grey blobs represent the struck portion of the QGP (scattering center), and its size represents the volume over which the exchanged gluon field is correlated with the plasma. The locations beyond this region will not be correlated. Thus, the energy loss of the hard parton is primarily controlled by the transport coefficient \( \hat{q} \) and follows \( \Delta E \propto \hat{q}L^2 \).

In the remainder of this chapter, we would refer the struck portion of the QGP as a “QGP degree of freedom” (QGP-DOF). Keeping the above assumptions in mind, we develop a new formulation of \( \hat{q} \) and demonstrate that \( \hat{q} \) can be expressed in terms of a PDF which gives rise the scale resolution dependence. The PDF, in this case, would refer to the momentum distribution of quasi-particle inside the QGP-DOF. We shall perform a model-to-data comparison of high-\( p_T \) hadron-\( R_{AA} \) to extract the possible forms of the quasi-particle distribution function of the QGP-DOF. In the end, we will show that scale evolution of \( \hat{q} \) provides a satisfactory explanation of the enhancement of \( \hat{q}/T^3 \) at RHIC collision energies relative to LHC collision energies.

### 4.2 Scale dependence of \( \hat{q} \)

We study here, in a boosted frame, the propagation of an energetic hard quark through a section of QGP where the hard quark carries momentum \( q = [0, q^- , 0] \) and the section of QGP carries momentum \( P_A = [P_A^+, 0, 0] \). Assuming in the limit of high energy (hard parton), the scattering within the plasma are independent, the scattering can thought to be from the QGP-DOF that carries momentum \( P = [P^+, 0, 0] \). The light-cone momenta \( q^- \),
Figure 4.1: High energy partons can be used to probe the very short-distance structure of QGP. The structure of QGP as seen by the hard parton in the limit of high energy and high-virtuality of the hard parton.

\( P_A^+ \) and \( P^+ >> 1 \text{ GeV} \).

We are interested in obtaining the expression of \( \hat{q} \) defined as average squared momentum broadening per unit length due to single scattering:

\[
\hat{q} = \frac{\langle \vec{k}_\perp^2 \rangle}{L} = \int \frac{d^2 k_\perp \vec{k}_\perp^2}{(2\pi)^2 L} \times \frac{d^2 W(\vec{k}_\perp)}{d^2 k_\perp}, \tag{4.1}
\]

where \( k \) is the momentum gain or lost by the hard quark in the scattering with the medium, and \( W(\vec{k}_\perp) \) represents the probability for the outgoing hard parton to carry the momentum.
\(q + k\). Here, \(L^4\) would represent a 4-D space-time volume of the box which contains a section of the QGP.

In general, one can obtain the transition probability for scattering processes at LO and NLO by considering terms at \(O(g^4)\) and \(O(g^6)\) in the expansion of following equation:

\[
W(k) = \text{Disc} \left[ \frac{1}{2N_c} \langle q^-, P_A | T \left\{ e^{-i \int_0^t dt H_I(t)} \right\} | q^-, P_A \rangle \right] \tag{4.2}
\]

where we have included factors from the average over initial color and spin of the quark. In above Eq. \(4.2\), \(T\) represents time ordering, \(H_I(t) = \int d^3x \bar{\psi}(x) i g \gamma^\mu t^a A^a_\mu \psi(x)\) represents the interacting Hamiltonian, and \(|P_A \rangle\) represents a QGP nuclear state. We show the leading order (LO) and next-leading order (NLO) diagrams to be taken into account for the evaluation of \(\hat{q}\) in Fig. \(4.2\) and \(4.3\).

We use the Cutkosky’s rules [84] to evaluate the amplitude square of a scattering process. The dotted line represents the cut-line, with a part on the left-hand side is the amplitude, and a part on the right-hand side is the complex conjugate of the scattering process. The cut line represents that the parton is on-shell, and we replace it’s propagator in Feynman amplitude \(1/(q_2^2) \rightarrow -2\pi i \delta(q_2^2)\). We shall perform our calculation in a finite box with volume \(V = L^3\) and in \(A^- = 0\) light-cone gauge, with a fixed light-cone vector \(n^\mu = [1, 0, 0, 0]_\perp\).

![Diagram](image-url)
Figure 4.3: Forward scattering diagrams at NLO contributing to $\hat{q}$. These are real diagrams with quark pdf. The dotted line represents the cut-line. The red blob represents a QGP degree of freedom with light-cone momentum $P = [P^+, 0, 0]$. 
4.2.1 Leading order expression of $\hat{q}$

First, we consider leading order diagram (at leading-twist) in which the hard quark ($q$) scatters off from a quark ($p$) in the QGP by exchanging a Glauber gluon ($k$). For this process, the forward scattering diagram is shown in Fig. 4.2. The shaded red blob, together with the attached quark-line, represents the non-perturbative quark pdf. A similar diagram exists for the gluon pdf. The transition probability for this process is given as

$$W_{LO} = \frac{g^4}{(2\pi)^4} \left[ \frac{1}{2N_c} \frac{1}{\sqrt{2E_qV}} \right] \int \frac{d^4k'}{d^4k} \int \frac{d^4q_2}{d^4q_1} \int \frac{d^4p_2}{d^4p_1} \int d^4z_3 d^4z_4 d^4z_0 d^4z_1 \text{Tr}[q^\rho \bar{q}_2^\gamma]$$

$$\times \text{Tr}[t^j t^i] \delta^{nj} \delta^{mi} d_{\rho \nu}(k') d_{\sigma \mu}(k) \left\langle P_A | \bar{\psi}(z_4) \gamma^\nu \bar{q}_2^\gamma \psi(z_3) | P_A \right\rangle \text{Tr} [t^m t^n]$$

$$\times e^{iz_0(q_2 - k)} e^{iz_1(q - k') - q_2} e^{-iz_4(p_2 - k')} \frac{1}{k^2 k'^2} \delta(q_2^2 - p_2^2).$$

(4.3)

where $|P_A\rangle$ represents a nuclear state with momentum $P_A = [P_A^+, 0, 0]$ which contains QGP degree of freedoms.

Note, we have used the on-shell condition for the two cut-lines, and hence replaced the propagator $\frac{1}{q_2^2} \rightarrow -2\pi i \delta(q_2^2)$, and $\frac{1}{p_2^2} \rightarrow -2\pi i \delta(p_2^2)$. Also, we have incorporated a factor of $\sqrt{2E_qV}$ in the denominator, which comes from the “box-normalization” for each external parton line, where $E = \sqrt{2q^-}$ and $V$ is the spatial volume of the box. To simplify the above expression, we perform $d^4z_0$ and $d^4z_1$ integration to get $\delta^4(q_2 - q + k) \delta^4(q - k' - q_2)$. Now, we introduce a new variable $p$ and $p'$ to shift the gluon momentum $k = -p + p_2$, $k' = -p' + p_2$. This makes $d^4k d^4k' = d^4pd^4p'$, $\delta^4(q_2 - q + k) = \delta^4(q_2 - q - p + p_2)$, and $\delta^4(q - k' - q_2) = \delta^4(q + p' - p_2 - q_2)$.

We evaluate the diagram in Glauber limit where gluon’s momentum $k \sim [\lambda^2, \lambda^2, \lambda]Q$, hard parton energy $q^-, P^+, p^+ \sim Q$. We perform $d^4p'$, $dp_2^+$, $d\vec{q}_2$, and $dp_2$ integration which
sets $q_2^- = q^-$, and $p_2^+ = p^+$. From the on-shell condition for final state partons we can write
\[
\delta(q_2^+ - \frac{q^+}{2q^-}) = \delta(p_2^+ - \frac{p^+}{2p^-}) = \delta(p_2^- - \frac{p^+}{2p^-}) = \frac{\delta(q^+_2 - q^-_2)}{2q^-} = \frac{\delta(p^+_2 - p^+_2)}{2p^+}.
\] (4.4)

This facilitates one to perform $dq^+_2$ and $dp^-_2$ integration. Thus, we have $p' = p$, $k' = k$, $q_2^+ = q^+$, and $p_2^- = p^+ + k^+$, $q_2^- = \frac{q^+}{2q^-}$, and $p_2^+ = \frac{p^+}{2p^-}$.

Now, we translate $z_3$ and $z_4$ in terms of their average and relative distances as
\[
z_4 = z + \frac{\Delta z}{2}; z_3 = z - \frac{\Delta z}{2}.
\] (4.5)

Thus, we can write
\[
\int d^4zd^4(\Delta z)dp^+dp^-d^2p_\perp e^{-i\Delta z p} \langle P_A | \bar{\psi}(z + \frac{\Delta z}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(z - \frac{\Delta z}{2}) | P_A \rangle \\
= \int d^4zd^4(\Delta z)dp^+(2\pi)^3\delta(\Delta z^+)\delta^2(\Delta z_\perp) e^{-i\Delta z^- p^+} \langle P_A | \bar{\psi}(z + \frac{\Delta z}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(z - \frac{\Delta z}{2}) | P_A \rangle \\
= \int d^4zd(\Delta z^-)dp^+(2\pi)^3e^{-i\Delta z^- p^+} \langle P_A | \bar{\psi}(z + \frac{\Delta z}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(z - \frac{\Delta z}{2}) | P_A \rangle.
\] (4.6)

The integration over $dp^-$ and $d^2p_\perp$ in second last line of Eq. (4.6) sets $\Delta z^+ = 0$ and $\Delta z_\perp = 0$, where we assumed the integrand to be a weak function of $p^-$ and $p_\perp$. Note that the final expression in Eq. (4.6) involves a nuclear state $|P_A\rangle$.

We convert a QGP nuclear state $|P_A\rangle$ into a corresponding internal DOF state $|P\rangle$ by employing results from Ref. [85]:
\[
\int d^4zd(\Delta z^-)e^{-i\Delta z^- p^+} \langle P_A | \bar{\psi}(z + \frac{\Delta z}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(z - \frac{\Delta z}{2}) | P_A \rangle \\
= \int d^4zd(\Delta z^-)\rho(z^-, z_\perp) \langle P | \bar{\psi}(z + \frac{\Delta z}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(z - \frac{\Delta z}{2}) | P \rangle \\
= \int d^4zd(\Delta z^-)\rho(z^-, z_\perp) \langle P | \bar{\psi}(\frac{\Delta z^-}{2})\gamma^\mu \not{p}_2 \gamma^\nu \psi(-\frac{\Delta z^-}{2}) | P \rangle.
\] (4.7)

where density $\rho(z^-, z_\perp)$ refers to the number of partons per unit volume inside the QGP at
location \((z^-, z_\perp)\) and \(P^+\) is the light-cone momentum of the QGP degree of freedom. Note, in the last line of Eq. [4.7], we have used the property of translational invariance of the inner product along a \(z\)-direction (4-D vector in a Minkowski space).

Putting all this together, we arrive at the following expression:

\[
W_{LO} = \left[ \frac{g^2 Tr[\gamma^\rho \gamma^\sigma] Tr[t^j t^i]}{4\sqrt{2} N_c V(q^-)^2} \right] \left[ \int \frac{d^2 k_\perp}{(2\pi)^2 k_\perp^4} \delta^{nj} \delta^{mi} d_{\rho\nu}(k) d_{\sigma\mu}(k) \right] \times \left[ \frac{g^2}{2\pi} \int \frac{dp^+}{2\pi} \int d^4zd(\Delta z^-) e^{-i\Delta z^- p^+} \frac{p(z^-, z_\perp)}{2P^+} \left\langle P \left| \bar{\psi} \gamma^n \gamma^\rho \gamma_2 \gamma^\mu \psi (-\frac{\Delta z^-}{2}) \right| P \right\rangle \right]
\]

First quantity in the bracket represents the contribution from the top quark line, second quantity represents the two Glauber gluons contribution to the amplitude, whereas the third bracket represents the bottom part of the diagram (Fig. 4.2). We study the process in the \(A^- = 0\) light-cone gauge, with light-cone vector \(n^\mu = [1, 0, 0, 1]\). We isolate the leading part as

\[
Tr[\gamma^\rho \gamma^\sigma] d_{\rho\nu}(k) d_{\sigma\mu}(k) = Tr[\gamma^\rho \gamma^\sigma] \left[ \frac{k_{\perp \nu} n_\rho}{k^-} \right] \left[ \frac{k_{\perp \mu} n_\sigma}{k^-} \right].
\]

We note that

\[
k^- = p_2^- = \frac{p_2^2}{2 p_2^+} = \frac{k_\perp^2}{k^-} = \frac{k_\perp^2}{2 xP^+},
\]

where momentum fraction \(x = \frac{p_2^+}{P^+}\). We make the leading twist approximation for \(\psi \bar{\psi} = pT \longrightarrow p^+ \gamma^- T\) to get \(T = \frac{T[\gamma^+ \gamma^- \psi \bar{\psi}]}{4p^+}\). Thus, we can write \(\psi \bar{\psi} = \frac{\gamma^-}{2} Tr \left[ \frac{\gamma^+ \gamma^- \psi \bar{\psi}}{2} \right] = \frac{\gamma^-}{2} Tr \left[ \psi \bar{\psi} \frac{\gamma^-}{2} \right].\)
Now, we can simplify

\[
\langle P \bar{\psi}(\frac{\Delta z^-}{2}) \gamma^\nu \gamma_2 \gamma^\mu \psi(-\frac{\Delta z^-}{2}) | P \rangle = \langle P \bar{\psi}(\frac{\Delta z^-}{2}) \gamma^+ \gamma_2 \gamma^\mu \psi(-\frac{\Delta z^-}{2}) | P \rangle \\
\times Tr \left[ \frac{\gamma^\nu}{2} \gamma_2 \gamma^\mu \right] \\
= \langle P \bar{\psi}(\frac{\Delta z^-}{2}) \gamma^+ \gamma_2 \gamma^\mu \psi(-\frac{\Delta z^-}{2}) | P \rangle \\
\times \left[ -g^\mu\nu \right] \frac{\vec{k}^2}{xP^+}. \tag{4.11}
\]

Let us now focus on the overall color factor given as

\[
Tr[t^j t^i] Tr[t^n t^m] \delta^{nj} \delta^{mi} = \frac{1}{4} \sum_{m=1}^{8} \delta^{mm} = \frac{C_F N_C}{2}. \tag{4.12}
\]

Finally, we arrive at the following expression:

\[
W_{LO} = \left[ g^4 \frac{C_F}{2\sqrt{2}} \right] \int_{\vec{k}_{\min}^2}^{Q^2} \frac{d\vec{k}_\perp^2}{(2\pi)\vec{k}_\perp^2} \int_\xi^{\xi+L} d\xi^- \rho(\xi^-) \int_{\vec{k}_\perp^2}^{\frac{\vec{k}_\perp^2}{2q^-P^+}} dx G_{QGP}^q(x), \tag{4.13}
\]

where \( G_{QGP}^q(x) \) is a quark-PDF inside QGP medium given as

\[
G_{QGP}^q(x) = \int \frac{d(\Delta z^-)}{2\pi} e^{-i\Delta z^- xP^+} \left\langle P \bar{\psi}(\frac{\Delta z^-}{2}) \gamma^+ \gamma_2 \gamma^\mu \psi(-\frac{\Delta z^-}{2}) | P \right\rangle. \tag{4.14}
\]

In Eq. 4.13, the upper limit of the transverse momentum of Glauber gluon \( \vec{k}^2_\perp \) can be taken either to be kinematic bound \( 2q^-P^+ \) or the scale \( Q^2 \) up to which the medium-modified fragmentation function is evolved. We define \( k_{\min} > \Lambda_{\text{QCD}} \) above which the pQCD is applicable. The light-cone coordinate \( \xi \) represents a location of the scattering of hard parton with a section of the QGP. We find that the lower bound for the momentum fraction \( x \) is set by \( \frac{k^+}{P^+} = \frac{\vec{k}^2}{2q^-P^+} \).
Thus, we can write the $\hat{q}$ at LO as

$$\hat{q}_{\text{LO}} = \left[ \frac{g^4}{2\sqrt{2}L} C_F \right] \int_{k^2_{\text{min}}}^{Q^2} \frac{d\vec{k}^2_1}{(2\pi)^2} \int_0^\xi \int_0^1 \int_0^{\sqrt{2} \rho(z^-)} \int_{\frac{\vec{k}^2_1}{2q^-p^+}}^1 dxG^q_{\text{QGP}}(x).$$

(4.15)

To understand how scale dependence arises in $\hat{q}$, we shall consider NLO diagrams.

4.2.2 NLO diagram: collinear emission in initial state

We consider here a next-leading order diagram contributing to $\hat{q}$, which involves emission of a gluon collinear to initial state target-like parton. For the forward scattering diagram shown in Fig. 4.3a, we employ optical theorem and compute the transition probability given as

$$W_{\text{NLO}(a)} = \frac{g^6}{(2\pi)^9} \left[ \frac{1}{2N_c \sqrt{2E_qV \sqrt{2E_qV}}} \right] \int d^4q_2d^4k'd^4k_1d^4l_3d^4p_2d^4l_1d^4l_2 \int d^4z_3d^4z_4$$

$$\times Tr[t^j t^i] \delta^{jm} \delta^{ni} \delta^4(q - q_2 - k) \delta^4(q_2 - q + k') \delta^4(k + l_1 - p_2) \delta^4(k' + l_3 - p_2)$$

$$\times \delta(q_2^2) \delta(p_2^2) \delta(l^2) Tr[\not{q} \not{g} \not{q} \not{g}] d_{\sigma\mu}(k)d_{\rho\nu}(k')d_{\alpha\beta}(l) \frac{1}{k^2k_1^2l_1^2l_3^2} \delta^{ab} Tr[t^b t^n t^m t^a]$$

$$\times \left\langle P_A \left| \bar{\psi}(z_3) \gamma^\beta P_3 \gamma^\mu \not{q}_2 \gamma^\alpha P_1 \bar{\psi}(z_3) \right| P_A \right\rangle e^{i z_3(l_1 + l)} e^{-i z_4(l_3 + l)} ,$$

(4.16)

where $|P_A\rangle$ represents a nuclear state with momentum $P_A = [P_A^+,0,0]$ which contains QGP degree of freedoms.

Note, we have used the on-shell condition for final state partons, and hence replaced their propagators $\frac{1}{q^2} \rightarrow -2\pi i\delta(q^2_2)$, $\frac{1}{p^2} \rightarrow -2\pi i\delta(p^2_2)$, and $\frac{1}{l^2} \rightarrow -2\pi i\delta(l^2)$. Also, we have incorporated a factor of $\sqrt{2E_qV}$ in the denominator which comes from the "box-normalization" for each external parton line, where $E = \sqrt{2q^-}$ and $V$ is the spatial volume of the box. Next, we do the space-time integral at vertex $z_{00}, z_{11}, z_1$, and $z_2$. We define $x' = \frac{p^+}{p^-}$ and follow similar algebraic manipulation used in section 4.2.1 to reduce Eq. 4.16.
to the following form:

\[
W_{\text{NLO}}(a) = \left[ g^2 \text{Tr}\left[\gamma^\mu \gamma_2 \gamma^\sigma\right] \text{Tr}\left[ t^i t^j \right] \right] \left[ \frac{d^2 k_\perp}{(2\pi)^2 k_\perp^4} \delta^{ni} \delta^{mi} d_{\rho\sigma}(k) d_{\sigma\mu}(k) \right] \\
\times g^4 \int \frac{d^2 l_\perp}{(2\pi)^4} \int d(\Delta z) \int \frac{d^4 z}{(2\pi)^4} \frac{\rho(z, z')}{2P^+} e^{-i\Delta z x' P^+} \left\langle P \left| \bar{\psi} \left( \frac{\Delta z^-}{2} \right) \gamma^\gamma \gamma^\beta \gamma^\mu \right| P \right\rangle \\
\times \delta^{ab} \text{Tr}\left[ t^b t^a t^m t^n \right] \text{Tr}\left[ \gamma^- \gamma^\beta f_3 \gamma^\nu \gamma_2 \gamma^\mu f_1 \gamma^\alpha \right] d_{\alpha\beta}(l) \left[ \frac{P^+ y}{8(1 - y)x' P^+ l_\perp^4} \right]. 
\]

(4.17)

where collinear emitted gluon carries momentum fraction \( y = \frac{l^+}{p^+} \) and transverse momentum \( \vec{l}_\perp \).

We can workout the color factor as

\[
\text{Tr}\left[ t^j t^i \right] \delta^{nj} \delta^{mi} \text{Tr}\left[ t^b t^m t^n t^a \right] \delta^{ab} = \frac{1}{2} \text{Tr}\left[ t^a t^a t^a t^a \right] = \frac{C_F N_c}{2} C_F. 
\]

(4.18)

We evaluated this diagram and found that the most dominant contribution comes from a region of the phase-space where transverse momentum of the collinear gluon emitted has \( |\vec{l}_\perp| << |\vec{k}_\perp| << q^- P^+ \). To isolate such leading poles, we define a hard scale \( \mu^2 \) such that \( |\vec{l}_\perp|^2 << \mu^2 \leq |\vec{k}_\perp|^2 \). Now, we write \( \vec{k}_\perp = \vec{l}_\perp + \vec{p}_{2\perp} \approx \vec{p}_{2\perp} \) and

\[
k^- = p^- + l^- \approx \frac{\vec{k}_\perp^2}{2(1 - y)x' P^+}. 
\]

(4.19)
In leading pole approximation, we get

\[
W_{\text{NLO}(a)} = \left[ g^4 C_F \right] \frac{Q^2}{2\sqrt{2}} \frac{d{k^2_\perp}}{(2\pi)k^2_\perp} \frac{g^2}{2} \int_{0}^{\mu^2} \frac{dl^2_\perp}{(2\pi)l^2_\perp} \frac{1}{2} \int_{0}^{\frac{k^2}{2q-P^+}} dy \left[ C_F y \right] \]

(4.20)

\[
\times \int_{\xi}^{\xi+L} dz^- \rho(z^-) \int_{\frac{k^2}{2q-P^+(1-y)}}^{1} dx' G^q_{\text{QGP}}(x'),
\]

where \( G^q_{\text{QGP}}(x) \) is defined in Eq. 4.14.

In above Eq. 4.20, the upper limit of the transverse momentum \( k^2_\perp \) can be taken either to be kinematic bound \( 2q-P^+ \) or the scale \( Q^2 \) up to which the medium-modified fragmentation function is evolved. The light-cone coordinate \( \xi \) represents the location of the scattering of hard parton with the section of the QGP. We find that the lower bound for the momentum fraction \( x' \) is set by \( \frac{k^+}{P^+(1-y)} = \frac{k^2}{2q-P^+(1-y)}. \)

4.2.3 NLO diagram: collinear emission in final state

In this subsection, we consider another NLO diagram in which collinear gluon is emitted from the final state quark. Using the optical theorem, we calculate the transition probability for the process shown in Fig. 4.3b given as

\[
W_{\text{NLO}(b)} = \frac{g^6}{(2\pi)^9} \left[ \frac{1}{2N_c} \frac{1}{2E_q V} \right] \int d^4q_2 d^4k d^4k' d^4l_1 d^4l_3 d^4l_4 d^4p_2 \int d^4z_3 d^4z_4
\]

\[
\times Tr[t^j t^i] \delta^{jm} \delta^{ni} \delta^4(q_2 + k - q) \delta^4(q - q_2 - k') \delta^4(l_1 - l - p_2) \delta^4(l + p_2 - l_3)
\]

(4.21)

\[
\times \delta(q_2^2) \delta(p_2^2) \delta(l^2) Tr[t^\alpha t^\beta] d_{\sigma\mu}(k) d_{\rho\nu}(k') d_{\alpha\beta}(l) \frac{1}{k^2 k'^2 l_1^2 l_3^2} \delta^{ab} Tr[t^{n} t^{m} t^{l} t^{m}]
\]

\[
\times \left< P_A \bigg| \bar{\psi}(z_4) \gamma^\nu I_3 \gamma^\beta \phi_2^{\gamma} \gamma^\alpha I_1 \gamma^\mu \psi(z_3) \bigg| P_A \right> e^{iz_4(k' - l_3)} e^{iz_3(l_1 - k)}
\]

where \( |P_A\rangle \) represents a nuclear state with momentum \( P_A = [P_A^+, 0, 0] \) which contains QGP degree of freedoms.

Note, we have used the on-shell condition for final state partons, and hence replaced their propagators \( \frac{1}{q^2} \rightarrow -2\pi i\delta(q^2), \frac{1}{p^2} \rightarrow -2\pi i\delta(p^2), \) and \( \frac{1}{l^2} \rightarrow -2\pi i\delta(l^2). \) Also, we
have incorporated a factor of $\sqrt{2E_qV}$ in the denominator which comes from the “box-normalization” for each external parton line, where $E = \sqrt{2q^−}$ and $V$ is the spatial 3D volume of the box. Next, we integrate out the $z_{00}, z_{11}, z_1,$ and $z_2$ space-time variables and apply transformations similar to used in section 4.2.1. This reduces Eq. 4.21 into a form given as

$$W_{\text{NLO}}(b) = \left[ \frac{g^2 \text{Tr}[\bar{t}_j t_i] \text{Tr}[\bar{t}_i t_j]}{4\sqrt{2N_c}V(q^−)^2} \right] \left[ \int \frac{d^2k_\perp}{(2\pi)^2k_\perp^4} \delta^{n\bar{j}} \delta^{mi} d_{\rho\mu}(k)d_{\sigma\lambda}(k) \right] \delta^{ab} \text{Tr}[t^n t^a t^m]$$

$$\times g^4 \int \frac{d^2l_\perp dy dx'}{(2\pi)^4} \int d(\Delta z^−)d^4z\frac{\rho(z^−, z_1)}{2P^+} e^{−i\Delta z^−x'P^+} \left\langle P \left| \bar{\psi}(\frac{\Delta z^−}{2}) \gamma^μ x^P \psi(−\frac{\Delta z^−}{2}) \right| P \right\rangle$$

$$\times \text{Tr} \left[ \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \right] d_{\alpha\beta}(l) \left[ \frac{P^+}{8(1−y)x'^P} \left[ \frac{k_\perp^2}{2} + 2x'P + k^- \right] \right],$$

(4.22)

where collinear emitted gluon carries momentum fraction $y = \frac{l^+}{p^+}$, and transverse momentum $\vec{l}_\perp$.

The overall color factor for this diagram is given as

$$\text{Tr}[t^j t^i] \delta^{n\bar{j}} \delta^{m\bar{i}} \text{Tr}[t^n t^a t^m] \delta^{ab} = \frac{1}{2} \text{Tr}[t^a t^a t^a t^a] = \frac{C_F N_c}{2} C_F.$$  (4.23)

We evaluated this diagram and found that the most dominant contribution comes from a region of the phase-space where transverse momentum of the collinear gluon emitted has $|\vec{l}_\perp| << |\vec{k}_\perp| << q^−, P^+$. To isolate such leading poles, we define a hard scale $\mu^2$ such that $|\vec{l}_\perp|^2 << \mu^2 \leq |\vec{k}_\perp|^2$. Now, we write $\vec{k}_\perp = \vec{l}_\perp + \vec{p}_{2\perp} \approx \vec{p}_{2\perp}$ and

$$k^- = p^− + l^- \approx \frac{\vec{k}_\perp^2}{2(1−y)x'^P}.$$  (4.24)
On evaluating the amplitude square in leading pole approximation, we arrive at

\[ W_{\text{NLO}(b)} = \left[ \frac{g^4 C_F}{2\sqrt{2}} \right] \int_{\mu^2}^{Q^2} \frac{d\bar{k}_1^2}{(2\pi)\bar{k}_1^2} \frac{g^2}{2} \int_0^{\mu^2} \frac{d\bar{l}_1^2}{(2\pi)\bar{l}_1^2} \int_0^{1-\frac{\bar{q}^2}{2q^-P^+}} dy \left[ 2C_F \right] \]

\[ \times \int_{\xi_L}^{\xi_L+L} dz^- \rho(z^-) \int_{\frac{\bar{l}_1^2}{2q^-P^+(1-y)}}^1 dx' G_{\text{QGP}}^q(x'). \]  

(4.25)

In above Eq. 4.25, the upper limit of the transverse momentum \( \bar{k}_1^2 \) can be taken either to be kinematic bound \( 2q^-P^+ \) or the scale \( Q^2 \) up to which the medium-modified fragmentation function is evolved. The light-cone coordinate \( \xi \) represents the location of the scattering of hard parton with the section of the QGP. We find that the lower bound for the momentum fraction \( x' \) is set by \( \frac{k^+ - q^- - P^+ + (1 - y)}{P^+(1-y)} \).

4.2.4 NLO diagram: interference of initial state and final state collinear gluon

In this section, we compute the interference diagram shown in Fig. 4.3c using optical theorem. We can write the contribution to transition probability as

\[ W_{\text{NLO}(c)} = \frac{g^6}{(2\pi)^9} \left[ \frac{1}{2N_c \sqrt{2E_qV}} \right] \int d^4q_2 d^4k d^4k' d^4l_1 d^4l_3 d^4l_4 d^4p_2 \int d^4z_3 d^4z_4 \]

\[ \times T r[\gamma^t \gamma^t] \delta^{in} \delta^{mi} \delta^4(q_2 + k - q) \delta^4(l_1 + l_3 - p_2) \delta^4(k + l_1 - p_3) \delta^4(p_2 + l - l_3) \]

\[ \times \delta(q_2^2) \delta(p_2^2) \delta(t^2) T r[\gamma^\mu \gamma_2^\sigma] d_{\sigma\rho}(k) d_{\rho\sigma}(l) \frac{1}{k^2 k^n l_1^2 l_3^2} \delta^{ab} T r[t^n t^a t^m] \]

\[ \times \left\langle P_A \left| \bar{\psi}(z_4) \gamma^\mu I_3^\beta \gamma^\alpha \psi(z_3) \right| P_A \right\rangle e^{iz_4(k^- - l^-)} e^{iz_3(l^+ + t^+)}, \]  

(4.26)

where \( |P_A\rangle \) represents a nuclear state with momentum \( P_A = [P_A^+, 0, 0] \) which contains QGP degree of freedoms.

Note, we have used the on-shell condition for the cut-lines, and hence replaced the on-shell propagators \( \frac{1}{q^2} \rightarrow -2\pi i\delta(q_2^2), \frac{1}{p^2} \rightarrow -2\pi i\delta(p_2^2) \), and \( \frac{1}{t} \rightarrow -2\pi i\delta(t^2) \). We have also performed the space-time integration at vertex \( z_{00}, z_{11}, z_1, \) and \( z_2 \). We follow similar algebraic
manipulation used in section 4.2.1 to reduce Eq. 4.26 to the following form

\[
W_{\text{NLO}(c)} = \left[ \frac{g^2 \text{Tr}[g\gamma^\mu g_2^\gamma] \text{Tr}[t^jt^i]}{4\sqrt{2}N_c V(q^-)^2} \right] \left[ \int \frac{d^2k_\perp}{(2\pi)^2k_\perp^2} \delta^{nj} \delta^{mi} d_{\nu\mu}(k)d_{\sigma\mu}(k) \right] \delta^{ab} \text{Tr}[t^n t^m t^a] \\
g^4 \int \frac{d^2\vec{l}_\perp dydx'}{(2\pi)^4} \int d(\Delta z^-) d^4z \frac{4(1-y)x'P+\vec{l}_\perp^2}{2} \left[ \frac{\rho(z^-, z_\perp)\Delta z^- \gamma^+}{2} \right] \left[ \psi\left(\frac{\Delta z^-}{2}\right) \frac{\gamma^+}{2} \psi\left(-\frac{\Delta z^-}{2}\right) \right] P
\]

\[
\text{Tr} \left[ \gamma^- \gamma^\nu \gamma_3 \gamma^\beta \bar{p}_2 \gamma^\mu \gamma_1 \gamma^\alpha \right] d_{\alpha\beta}(l) \left[ \frac{-P^+}{8(1-y)x'P+\vec{l}_\perp^2} \right] \left[ -\vec{k}_\perp^2 + 2x'P+k^- \right],
\]

(4.27)

where collinear emitted gluon carries momentum fraction \(y = \frac{l_\perp}{p_\perp}\), and transverse momentum \(\vec{l}_\perp\).

The overall color factor for this diagram is given as

\[
\text{Tr}[t^jt^i] \delta^{nj} \delta^{mi} \text{Tr}[t^n t^m t^a] \delta^{ab} = \frac{1}{2} \text{Tr}[t^mt^m t^a] = \frac{C_F N_c}{2} \left[ C_F - \frac{N_c}{2} \right].
\]

(4.28)

We evaluated this diagram and found that the most dominant contribution comes from a region of the phase-space where transverse momentum of the collinear gluon emitted has \(|\vec{l}_\perp| << |\vec{k}_\perp| << q^-, P^+\). To isolate such leading poles, we define a hard scale \(\mu^2\) such that \(|\vec{l}_\perp|^2 << \mu^2 \leq |\vec{k}_\perp|^2\). Now, we write \(\vec{k}_\perp = \vec{l}_\perp + \vec{p}_{2\perp} \approx \vec{p}_{2\perp}\) and

\[
k^- = p_2^- + l^- \approx \frac{\vec{k}_\perp^2}{2(1-y)x'P^+}.
\]

(4.29)

The expression \(W_{\text{NLO}(c)}\) (Eq. 4.27) in leading pole approximation can be recast into following
\[ W_{\text{NLO}(c)} = \left( \frac{g^4 C_F}{2\sqrt{2}} \right) \frac{Q^2}{\mu^2} \int_{\mu^2} d\frac{k^2}{2(2\pi)^2} \frac{g^2}{2} \int_{0}^{\nu^2} d\frac{l^2}{2(2\pi)^2} \int_{0}^{1} dy \left( \frac{N_c}{2} - C_F \right) \int_{\xi}^{\xi+L} dz \rho(z^-) \]

\[ \times \int_{\frac{k^2}{2q^-P^+}}^{1} dx' G^q_{\text{QGP}}(x'). \]

(4.30)

In above Eq. (4.30) the upper limit of the transverse momentum \( \tilde{k}^2_1 \) can be taken either to be the kinematic bound \( 2q^-P^+ \) or the scale \( Q^2 \) up to which the medium-modified fragmentation function is evolved. The light-cone coordinate \( \xi \) represents the location of scattering of hard parton with the section of the QGP. Here, \( L \) represents length of the section of the QGP.

We find that the lower bound for the momentum fraction \( x' \) is set by \( \frac{k^+}{P^+(1-y)} = \frac{\tilde{k}^2_1}{2q^-P^+(1-y)}. \)

We note that the diagram shown in Fig. 4.3d gives forward scattering amplitude identical to the one given in Eq. (4.27). Therefore, the contribution of the diagrams (Fig. 4.3c and 4.3d) are identical, hence, we would not present the detailed calculations for the diagram (4.3d).

4.2.5 NLO diagram: interference diagram with a three-gluon vertex

Next, we consider an interference diagram which involves a three-gluon vertex. For this process, the amplitude square is evaluated by constructing a forward scattering diagram shown in Fig. 4.3e. Using the optical theorem we write transition probability as

\[ W_{\text{NLO}(e)} = -\frac{ig^6}{(2\pi)^3} \left[ \frac{1}{2N_c} \sqrt{\gamma V} \frac{1}{\sqrt{\gamma V}} \right] \int d^4q_2 d^4k d^4k' d^4l_1 d^4l_3 d^4p_2 \int d^4z_3 d^4z_4 \]

\[ \times Tr[t^j t^i] \delta^{j\alpha} \delta^{\alpha\beta} d^4\gamma d^4\delta \left[ g^\mu(k + l) \gamma^\nu l_1 \gamma^\beta l_3 + g^\nu(k + l) \gamma^\mu l_1 \gamma^\beta l_3 \right] \]

\[ \times d_{\alpha\beta}(l_1) d_{\beta\gamma}(l) f^{mdc} \left[ g^{\mu\nu}(k + l) + g^{\nu\xi}(l - l_1) + g^{\xi\mu}(l_1 - k) \right] \]

\[ \times \left( P_A \bar{\psi}(z_4) \gamma^\nu f_3 \gamma^\beta \phi_2 \gamma^\alpha \psi(z_3) \right) \left( \bar{P}_A \gamma^\nu f_3 \gamma^\beta \phi_2 \gamma^\alpha \psi(z_3) \right) e^{i \frac{1}{2} (2P_2 + p_2)} (2P_2 + 1), \]

(4.31)
where \(|P_A\rangle\) represents a nuclear state with momentum \(P_A = [P_A^+, 0, 0]\) which contains QGP degree of freedoms.

Note, we have used the on-shell condition for final state parton, and hence replaced their propagators \(\frac{1}{q^2} \rightarrow -2\pi i\delta(q^2)\), \(\frac{1}{p^2} \rightarrow -2\pi i\delta(p^2)\), and \(\frac{1}{t^2} \rightarrow -2\pi i\delta(t^2)\). Also, we have incorporated a factor of \(\sqrt{2E_qV}\) in the denominator which comes from the “box-normalization” for each external parton line, where \(E = \sqrt{2q^–}\) and \(V\) is the spatial volume of the box. Next, we perform the space-time integration at vertex \(z_{00}, z_{11}, z_1,\) and \(z_2\) and apply similar algebraic manipulation used in section 4.2.1 to reduce Eq. 4.31 into a following form

\[
W_{NLO(e)} = \left[ \frac{g^2 Tr[\gamma^\rho \bar{q}_2 \gamma^\sigma Tr[t^j t^i]]}{4\sqrt{2}N_c V(q^-)^2} \right] \left[ \int \frac{d^2k_{\perp}}{(2\pi)^2 k_{\perp}^4} \delta^{nj}\delta^{mi} d_{\mu\nu}(k) d_{\sigma\mu}(k) \right] \\
\times g^4 \int \frac{d^2p_{2\perp} dp_{2\perp}}{(2\pi)^4} \int d(\Delta z^-) d^4z \frac{\rho(z^-, \Delta z^-)}{2P^+} e^{-i\Delta z^- x^+ P^+} \left\langle P \left| \bar{\psi}(\Delta z^-) \gamma^+ \psi(-\Delta z^-) \right| P \right\rangle \\
\times (-i)^{mde} \left[ g^{\mu\sigma}(k + l)^\xi + g^{\xi\epsilon}(-l - l_1)^\mu + g^{\xi\epsilon}(l_1 - l)^\epsilon \right] \\
\times \delta^{ac}\delta^{db} Tr[t^n t^b t^a] Tr \left[ \gamma^- \gamma^\nu I_3 \gamma^\beta \bar{q}_2 \gamma^\alpha \right] d_{\alpha\epsilon}(l_1) d_{\epsilon\beta}(l) \left[ \frac{P^+}{8(1 - y) y x^+ P^+ l_{2\perp}^2} \right],
\]

(4.32)

where emitted gluon in the final state carries the momentum fraction \(y = \frac{l_{2\perp}^+}{P^+}\), and the transverse momentum \(\vec{l}_{\perp}\). The final state quark collinear to target carries the transverse momentum \(\vec{p}_{2\perp}\).

The overall color factor for this diagram is given as

\[
Tr[t^j t^i] \delta^{nj}\delta^{mi} f^{mde} Tr[t^n t^b t^a] \delta^{db}\delta^{ac} = \frac{\delta^{ji}}{2} \frac{i N_c}{2} Tr[t^j t^i] = \frac{C_F N_c}{2} \left[ \frac{i N_c}{2} \right].
\]

(4.33)

We evaluated this diagram and found that the most dominant contribution comes from a region of the phase-space where \(|\vec{p}_{2\perp}| << |\vec{k}_{\perp}| << q^–, P^+\). To isolate such leading poles, we define a hard scale \(\mu^2\) such that \(|\vec{p}_{2\perp}|^2 << \mu^2 \leq |\vec{k}_{\perp}|^2\). Note that \(\vec{k}_{\perp} = \vec{l}_{\perp} + \vec{p}_{2\perp} \simeq \vec{l}_{\perp}\). Thus,
we can write

\[ k^- = p^- + l^- \simeq \frac{\vec{k}_\perp^2}{2yx'P^+}, \quad (4.34) \]

\[ l_1^2 = (p - p_2)^2 = -2x'P^+p^- = -\frac{\vec{p}_\perp^2}{(1 - y)}, \quad (4.35) \]

and

\[ l_3^2 = (k + p)^2 = -\vec{k}_\perp^2 + 2x'P^+k^- = \frac{(1 - y)}{y}\vec{k}_\perp^2. \quad (4.36) \]

On simplifying the expression (Eq. 4.32) in leading pole approximation, we arrive at the following expression

\[
W_{NLO(e)} = \left[ g^4 C_F \sqrt{2} \right] \int_{\mu^2}^{Q^2} \frac{d\vec{k}_\perp^2}{(2\pi)\vec{k}_\perp^2} \int_0^{1-\frac{\vec{k}_\perp^2}{2q^-P^+}} dy \int_0^{\frac{\vec{p}_\perp^2}{(2\pi)\vec{p}_\perp^2}} dp_\perp^2 \left[ -\frac{N_c}{2} \right] \int_{\xi}^{\xi+L} dz^- \rho(z^-) \\
x \int_{\frac{\vec{k}_\perp^2}{2q^-P^+}}^{1} dx' G_{QGP}(x'). \quad (4.37)
\]

In above Eq. 4.37 the upper limit of the transverse momentum \( \vec{k}_\perp^2 \) can be taken either to be the kinematic bound \( 2q^-P^+ \) or the scale \( Q^2 \) up to which the medium-modified fragmentation function is evolved. The light-cone coordinate \( \xi \) represents the location of scattering of hard parton with the section of the QGP. We find that the lower bound for the momentum fraction \( x' \) is set by \( \frac{k^+}{P^+(1-y)} = \frac{\vec{k}_\perp^2}{2q^-P^+(1-y)}. \)

If one work out the forward scattering amplitude for the diagram shown in figure 4.3f, one finds that it is identical to the one given in Eq. 4.32. Therefore, the contribution of both diagrams (Fig. 4.3e and 4.3f) are identical, hence, we would not present the detailed calculations for the diagram shown in Fig. 4.3f.
4.2.6 Summation of NLO real diagrams with quark pdf

We can sum the contributions from the NLO diagrams shown in Fig. 4.3 to get the transition probability at NLO as

\[
W_{NLO} = \left[ g^4 \frac{C_F}{2\sqrt{2}} \right] \int \frac{d\vec{k}_\perp^2}{(2\pi)k_\perp^2} \frac{g^2}{2} \int \frac{d\vec{l}_\perp^2}{(2\pi)l_\perp^2} \int dy \left[ C_F y + \frac{2C_F}{y} + 2 \left( \frac{N_c}{2} - C_F \right) - 2 \frac{N_c}{2} \right] \\
\times \int_\xi^{\xi+L} dz^- \rho(z^-) \int \frac{1}{\xi^3} \frac{d\vec{x}'}{2\xi^2 P^+(1-y)} \int dx' C_F \left[ \frac{1 + (1 - y)^2}{y} \right] C_F \int z^- \rho(z^-) \\
\times \int \frac{1}{\xi^3} \frac{d\vec{x}'}{2\xi^2 P^+(1-y)} G_{QGP}'(x'),
\]

where \( x' = \frac{p^+}{P^+} \). Now, we define a momentum fraction \( x = x'(1 - y) \) to represent the ratio of a momentum carried by the parton after splitting relative to the momentum \( P^+ \) of the QGP degree of freedom. This gives

\[
W_{NLO} = \left[ g^4 \frac{C_F}{2\sqrt{2}} \right] \int \frac{d\vec{k}_\perp^2}{(2\pi)k_\perp^2} \frac{g^2}{2} \int \frac{d\vec{l}_\perp^2}{(2\pi)l_\perp^2} \int dx \int_0^{1-x} dy \left[ \frac{1 + (1 - y)^2}{1 - y} \right] C_F \\
\times \int_\xi^{\xi+L} dz^- \rho(z^-) \times G_{QGP}' \left( \frac{x}{1 - y} \right).
\]

(4.39)
Thus, \( \hat{q} \) at NLO is given as

\[
\hat{q}_{\text{NLO}} = \left[ \frac{g^4}{2\sqrt{2}L} C_F \right] \int_{\mu^2}^{Q^2} d\vec{k}_\perp^2 \frac{g^2}{(2\pi)^2} \frac{d^2l_\perp}{(2\pi)^2} \int_{\xi^2}^{\xi+L} dx \int_{1-x}^{1-y} dy \left[ \frac{1 + (1-y)^2}{y} \right] C_F \\
\times \int_{\xi}^{\xi+L} dz^- \rho(z^-) \times G_{QGP}^q \left( \frac{x}{1-y} \right),
\]

(4.40)

where quantity \([\frac{(1 + (1-y)^2)}{y}]\) represents the splitting function for a quark to emit a gluon with momentum fraction \(y\). Note, the integrand \(\int \frac{d^2l_\perp}{\mu^2}\) has no ultraviolet divergence, because \(|\vec{l}_\perp|^2 < \mu^2 \leq |\vec{k}_\perp|^2 \leq 2q^-P^+\), but has an infrared divergence as \(|\vec{l}_\perp| \to 0\). We also note that the term \(g^2 \int \frac{d^2l_\perp}{\mu^2} \sim 1\) appear as a resum parameter.

One can consider a series of higher-order diagrams with multiple gluon emissions collinear to quarks in the medium, and resum \(\hat{q}\) to a finite value by absorbing the infrared divergent part \(\int \frac{d^2l_\perp}{\mu^2} \to \int \frac{d^2l_\perp}{\mu^2} + \int \frac{d^2l_\perp}{\mu^2} \) into a redefinition of the QGP-PDF. This transformation makes QGP-PDF \(G_{QGP}(x, \mu^2)\) a scale dependent object, and thereby the transport coefficient \(\hat{q}\) acquires a scale dependence. Resuming the diagram in leading-pole approximation, we get a scale-dependent physical form of \(\hat{q}\) given as

\[
\hat{q}(\xi, q^-, \mu^2) = \left[ \frac{(4\pi)^2 C_F}{2\sqrt{2}L} \right] \int_{\mu^2}^{Q^2} d\vec{k}_\perp^2 \frac{C_F}{(2\pi)^2} \frac{d^2l_\perp}{(2\pi)^2} \int_{\xi}^{\xi+L} dz^- \rho(z^-) \int_{\xi}^{\xi+L} dx G_{QGP}(x, \vec{k}_\perp^2),
\]

(4.41)

where \(G_{QGP}(x, \vec{k}_\perp^2)\) represents the PDF of quasi-particles in the QGP degree of freedom at scale \(\vec{k}_\perp^2\).

Also, note that we have chosen \(k_{\text{min}}^2\) in Eq. 4.15 to be \(\mu^2 > \Lambda_{\text{QCD}}^2\). We can clearly see from Eq. 4.41 that transport coefficient \(\hat{q}\) depends not only on the local number density but also scale \(\mu\), and incident hard parton’s energy \(q^-\). This justifies our claim that \(\hat{q}\) depends on the resolution scale of the hard probe.
4.3 Computing $\hat{q}$ within phenomenological assumptions

In this section, we discuss phenomenological aspects involved in the calculation of scale-dependent $\hat{q}$. The first thing we point out is that the equation derived in the previous section (4.41) was under the assumption that transverse momentum ($k_\perp$) exchanged are above non-perturbative scale $\Lambda_{\text{QCD}}$ where the pQCD is valid. To determine the range of $k_\perp^2$ in the $\hat{q}$ integral, we recall the phenomenon of color coherence as discussed during the analysis of the medium-induced single emission diagram in Chapter 3, Sec. 3.3. Through Eq. 3.7, Eq. 3.8 and Fig. 3.2, it was shown that, for a given virtuality ($\mu^2$) of the hard quark, the transverse momentum of radiated collinear gluon $l_\perp^2 \approx \mu^2$ and the dominant range of $|\vec{k}_\perp|$ (transverse gluon) integral lies in $\mu \pm \mu/2$. We also discussed that as the virtuality ($\mu^2 \approx l_\perp^2$) increases, the range of $k_\perp^2$ that contributes to $\hat{q}$ also shifts to a higher interval.

In other words, we can say the gluons from the medium can resolve the dipole traversing the plasma if the size of the dipole is on the order of the wavelength of the gluon. This sets the scale of the $\hat{q}$ to be same as the scale of the medium-modified fragmentation function. Thus, the range of $k_\perp^2$ integration in $\hat{q}$ ranges from $\mu^2/4$ to $9\mu^2/4$. In realistic calculations of the single hadron $R_AA$ and $\nu_2$, the fragmentation function scale $\mu^2$ ranges from $p_T^2$ (detected-hadron) to 1 GeV$^2$.

To deal with this, we use two different methods. In method [A], we keep the range of the $k_\perp^2$ integration from $\mu^2/4$ to $9\mu^2/4$, but restrict the lower bound to be always above 1 GeV$^2$. The expression is given as

$$[A]: \hat{q}^{[A]}(\xi, q^-, \mu^2) = \left[\frac{(4\pi)^2C_F}{2\sqrt{2}L}\right] \int_{\mu^2/4}^{9\mu^2/4} \frac{dk_\perp^2}{(2\pi)^2k_\perp^2} \frac{\alpha_s^2(k^2)}{\xi^L_+} \int dz^- \rho(z^-) \int_1^1 dx G_{\text{QGP}}(x, k_\perp^2),$$

(4.42)

In the method [B], we keep the lower to be $\mu^2$ (scale of the fragmentation function) and take
the upper limit to be $9\mu^2$. The expression for this case is given as

$$\langle B \rangle : \hat{q}^{[B]}(\xi, q^-, \mu^2) = \left[ \frac{(4\pi)^2 C_F}{2\sqrt{2}L} \right] \int_{\mu^2}^{9\mu^2} \frac{d\vec{k}_\perp^2}{(2\pi)^2} \alpha_s^2(\vec{k}) \int_{\xi}^{\xi+L} \frac{dz}{\xi} \rho(z^-) \int_{\frac{\xi^2}{2q^-}p^+}^{1} dx G_{QGP}(x, \vec{k}_\perp^2),$$

(4.43)

It will be shown in the next sections that both methods provide a similar description to single-hadron $R_{AA}$ and $\nu_2$. Note, the above equations enable us to calculate the $\hat{q}/T^3$ that depends on the hard parton’s energy, and scale of the probe. But, before we proceed to demonstrate such computation, we want to address what we mean by PDF of QGP-DOF, and how do we define momentum fraction $x$ for the PDF. The QGP-DOF refers to the struck portion of the QGP over which the gluon fields are correlated. In the limit of high energy hard parton, all subsequent scatterings are not correlated with one another. This is one of the basic assumptions in calculations done using pQCD based jet quenching formalism. The underlying structure of the QGP-DOF could be in terms of quarks and gluon quasi-particles or some other kind of entities.

To define the momentum fraction $x$ carried by the quasi-particles inside the QGP-DOF, we boost to the rest frame of QGP. Thus, the $x$ for the quasi-particles is given by

$$x = \frac{k_\perp^2}{2EM}$$

(4.44)

where $k_\perp^2$ is the momentum of the transverse gluon, $E$ is the energy of the hard parton, and $M$ is the mass of the QGP-DOF in its rest-frame. It would certainly be true that the mass of QGP-DOF would be a function of the local temperature. Hence, we use estimates from finite-temperature field theory and find the mass of the enclosure containing the degree of the freedom to be $m_{DOF} \sim gT$, where $g$ is the bare coupling constant of the medium at the temperature $T$. So, if the temperature of the plasma $T \approx 400\text{MeV}$ and the strong coupling constant $\alpha_s = 0.3 \Rightarrow g \approx 2$, yield the mass to be $M \approx 800 \text{MeV}$. This enables us to estimate
the upper bound of the mass of the QGP-DOF (in the rest frame of the plasma) as \( gT \leq M_N \), where \( M_N \) is the mass of a nucleon (1 GeV). Like the scale evolution of proton’s PDF and fragmentation functions requires the knowledge of the distribution function at lower scale, the case of PDF of QGP-DOF is no different. The PDF of QGP-DOF at a lower scale \( \mu^2 = 1 \text{ GeV}^2 \) will be an input in the calculation of \( \hat{q} \) and PDF at higher scale will be obtained by DGLAP evolution.

In this first attempt, we parametrize the PDF using Feynman-Field form [86]:

\[
G_{\text{QGP}}(x, \mu^2 = 1\text{GeV}^2) = Nx^a(1 - x)^b.
\] (4.45)

The three coefficients \( N, a \) and \( b \) are not independent of each other: The choice of \( a \) and \( b \) restricts the choice of \( N \) and determined by the normalization constraint \( \int_0^1 dx x G_{\text{QGP}}(x, \mu^2 = 1\text{GeV}^2) = 1 \). The evolution of PDF is governed by rules of DGLAP equation given as

\[
\frac{\partial G(x, \mu^2)}{\partial \log \mu^2} = \frac{\alpha_s(\mu^2)}{2\pi} \int_x^1 \frac{dy}{y} G(y, \mu^2) P\left(\frac{x}{y}\right).
\] (4.46)

In our calculation, we assume the function \( P(x) = P_{gg}(x) \), where \( P_{gg} \) is the standard AP splitting function for the gluon with momentum fraction \( x \) coming off from another gluon in the plasma. We approximate \( G_{\text{QGP}}(x, \mu^2) \equiv G(x, \mu^2) \).

Note, in the above equation we have ignored the flavor-dependence. Extracting the flavor-dependent QGP-PDF would increase the number of fit parameters in our full phenomenological calculations and would be well suited for Bayesian statistical analysis to be done in future. In equations 4.42 and 4.43 to simplify the length integration, we average over an appropriate length traverse by the hard parton prior to emission denoted \( L \). This is typically the formation length of the radiation. We replace the \( \rho \) with average density as:

\[
\int_{\xi}^{\xi+L} dz^- \rho(z^-) = \int_{\xi}^{\xi+L} dz^- \rho_{\text{avg}}(\xi+L/2) = \rho_{\text{avg}}(\xi + L/2) = \frac{\hat{q}_0}{s_0} \frac{s}{s_0},
\] (4.47)
where $s$ is the average local entropy density, $s_0 = 96 \text{ fm}^{-3}$ and $\hat{q}_0$ is a dimensionless free parameter.

### 4.4 Resolution of JET collaboration $\hat{q}$ puzzle

In this section, we study explicitly the effects of scale dependence in transport coefficient $\hat{q}$. To do this, we obtain the expression of $\hat{q}/T^3$ by substituting Eq. 4.47 into Eq. 4.42 given as

$$
\frac{\hat{q}[A](\xi, E, \mu^2)}{T^3} = \hat{q}_0 \frac{s}{s_0 T^3} \left[ \frac{(4\pi)^2 C_F}{2\sqrt{2}} \int_{\mu^2/4}^{9\mu^2/4} \frac{d\vec{k}_\perp^2}{(2\pi)^2 k_\perp^2} \alpha_s^2(k_\perp^2) \int_{EM} dx G_{QGP}(x, \vec{k}_\perp^2) \right],
$$

(4.48)

The quantity within the square bracket is a new factor that encodes the scale and energy dependence of the hard parton. We compute the quantity within the square bracket (Eq. 4.48) and plot as a function of scale $\mu^2$ in Fig. 4.4(d). For a fixed given temperature (entropy density) and an overall normalization factor, this quantity is interaction strength $\hat{q}/T^3$.

The PDF used as input at $\mu^2 = 1 \text{ GeV}^2$ is shown in black solid line (Fig. 4.4)(a). We evolve the input PDF to higher scales using the DGLAP equation (Eq. 4.46). From Fig. 4.4(b), we observe that PDFs at a higher scale tend to follow a sea-like distribution. The integral $dx$ over QGP-PDF drops as the $\mu^2$ is increased. This is shown in Fig. 4.4(c) and is mainly due to a decrease in the lower limit of $x$ integral as the $\mu^2$ is increased. We observe from the plot (Fig. 4.4(d)) that the magnitude of $\hat{q}/T^3$ reduces as one goes to higher and higher scale $\mu^2$ for a given energy $E$ of the hard parton. This effect should be interpreted as a consequence of scaling violations similar to the one observed in the case of $e$-$p$ DIS experiments.

In relativistic heavy-ion collisions, the hard partons produced at LHC (hadron $p_T \sim 100 \text{ GeV/c}$) collision energies would sample the QGP medium with large $\mu^2$ gluons as compared to the hard partons produced at RHIC (hadron $p_T \sim 10 \text{ GeV/c}$) collision energies. Therefore, the hard partons have considerably higher virtuality at the LHC. This means the probes
are smaller in transverse size, and a section of QGP probed will appear more dilute. This essentially indicates that $\hat{q}/T^3$ at a fixed temperature is solely enhanced at RHIC due to scale evolution, and hence provides an explanation of the JET collaboration $\hat{q}$ puzzle discussed in Chapter 3, Sec. 3.5.

Moreover, this setup (Eq. 4.48) also allows us to directly compute the 4th-moment of
transverse momentum exchange, defined as $\langle k_\perp^4 \rangle / L^-$. We show the scale dependence of 4th-moment $\langle k_\perp^4 \rangle / L^-$ scaled by $\mu^2$ in Fig. 4.5(b). The input-PDF used at scale $\mu^2 = 1 \text{ GeV}^2$ is presented with the black line in Fig. 4.4. The fourth-order term arising from the twist expansion was highlighted in Eq. 3.11. Typically, these higher-order terms are ignored in all higher-twist calculations of energy loss. In this case, since we have an explicit model of $\hat{q}$ we demonstrate that these terms are, indeed, quite smaller than terms relative to $\langle k_\perp^2 \rangle / L^-$ which was only retained in the calculation. This is an a posteriori justification of the twist expansion carried out in Chapter 3 Section 3.3.

Figure 4.5: Scale evolution of $\hat{q}$ and 4th-moment of transverse momentum exchange $\langle k_\perp^4 \rangle / L^-$ for a fix given temperature (entropy density) and an overall normalization factor. The input PDF used at scale $\mu^2 = 1 \text{ GeV}^2$ is shown in Fig. 4.4(b) with black line. The hard parton energy $E = 50 \text{ GeV}$ (in the rest-frame of QGP-DOF).

In the next section, we demonstrate that the formulation of scale-dependent $\hat{q}$ indeed explains the single-hadron suppression at RHIC and LHC simultaneously without the need to re-adjust the free parameters.
4.5 Observables \( R_{AA} \) and \( \nu_2 \) calculations

To demonstrate the validity of the scale dependent formulation of \( \hat{q} \) described above, we compute single-hadron observables such as the nuclear modification factor \( R_{AA} \), and azimuthal anisotropy \( \nu_2 \) within the formalism of high-twist energy loss. The nuclear modification factor \( R_{AA} \) measures the differential yield of hadrons in nucleus-nucleus collision relative to expectation from the proton-proton collision scaled by the number of expected binary collision in the nucleus-nucleus collision.

\[
R_{AA}(p_T, b_{\text{min}}, b_{\text{max}}) = \frac{\frac{d\sigma^{AA}}{dyd^2p_T}(b_{\text{min}}, b_{\text{max}})}{T_{AA}(b_{\text{min}}, b_{\text{max}}) \frac{d\sigma^{pp}}{dyd^2p_T}}, \tag{4.49}
\]

where \( T_{AA}(b_{\text{min}}, b_{\text{max}}) = \int_{b_{\text{min}}}^{b_{\text{max}}} d^2b \tau dzdz' \rho_{A_1}(\vec{r} + \vec{b}/2, z) \rho_{A_2}(\vec{r} - \vec{b}/2, z') \) corresponds to the average number of nucleon-nucleon collision expected in nucleus-nucleus collision within the impact parameter \( b_{\text{min}} \) and \( b_{\text{max}} \).

We take \( z \)-axis to be along the beam direction, whereas vector \( \vec{b} \) and \( \vec{r} \) are in a plane transverse to the beam direction. We would perform our calculation for the jet going at \( \eta, y = 0 \). We compute \( R_{AA} \) for final state hard hadrons with transverse momentum \( p_T \geq 8 \) GeV (pQCD regime) produced in Au+Au collision (RHIC) at \( \sqrt{s} = 200 \) GeV per nucleon, and for Pb+Pb collision (LHC) at \( \sqrt{s} = 2.76 \) TeV per nucleon. To compute the differential cross section of high-\( p_T \) hadron for the case of \( p-p \) (Eq. 4.49), we use factorization theorem given in Eq. 3.1. We use vacuum fragmentation function at known scale \( \mu^2 = 1 \) GeV\(^2\) from Kniehl, Kramer, Potter (KKP) results Ref. [87–89]. The input proton-PDF used is from CTEQ collaboration [90]. The factorization scale is set to be \( Q^2 = p_T^2 \).

To compute the differential cross section of high-\( p_T \) in Eq. 4.49, we evaluate the equation 3.4. Initial state nuclear structure functions have been used from CTEQ collaboration [90] including nuclear shadowing [91] effects. The medium-modified fragmentation function have been calculated using an evolution equation 3.15 outlined in Chapter 3 section 3.4. We scale \( \rho(\xi) \) with the event-averaged local entropy density of the QGP at the location \( \xi \). To obtain
Figure 4.6: Nuclear modification factor $R_{AA}$ of hadrons based on higher-twist approach with a scale dependent $\hat{q}$ using prescription [A]. The QGP-PDF shown with blue dashed line in Fig. 4.10(c,d) is used as input PDF in scale evolution of $\hat{q}$.

the profile of local entropy density for the QGP, we use $2 + 1$ D viscous fluid dynamical simulation by OSU-group [76–78, 92]. Input parameters such as viscosity, components of the initial energy-momentum tensor, and final freezeout criteria are fixed using the best fit results for the spectra and elliptic flow of hadrons with $p_T \leq 2$ GeV. The QGP has been assumed to be thermalized at $\tau_0 = 0.6$ fm/c for both RHIC and LHC energies.

We employ initial conditions for the two colliding nuclei with saturated gluon distributions [32, 93] using the MC-KLN model [94]. The jets are assumed to be produced using binary
collision profile at collision time $t_0 = 0$. We assume that the soft medium remains unchanged from 0 to 0.6 fm/c. The jets are assumed to decouple from the medium when the local temperature of the QGP medium reaches 160 MeV. We create a space-time profile of $\hat{q}$ for jets traveling in all directions, starting at any location $\vec{r}$ in the medium, and vanishing when $T = 160$ MeV.

To constrain the free parameters, we compute hadron-$R_{AA}$ by performing a full model calculation where the scale-dependent $\hat{q}$ (Prescription [A], Eq. 4.48) is input to the medium-modified fragmentation function (Eq. 3.15). We use QGP-PDF $G_{QGP}(x, \mu^2 = 1 \text{ GeV}^2)$ at scale $\mu^2 = 1 \text{ GeV}^2$ as a global fit function. We vary parameters $a$, $b$ and $\hat{q}_0$ to obtain the best combined-fit at 0-5% centrality bin at LHC and the 0-10% centrality bin at the RHIC as they have smallest error bar (Fig. 4.6 plot on the bottom row). The QGP-PDF used in this calculation is sea-like and shown with dotted lines in Fig. 4.10. It is visible that the simultaneous description of hadron-$R_{AA}$ at RHIC and LHC most central collisions is reasonably good. We are able to obtain a good description without having to readjust the parameters between RHIC and LHC energies.

Now, we fix the parameters $a$, $b$ and $\hat{q}_0$ and compute hadron-$R_{AA}$ for three different semi-peripheral collisions at RHIC and LHC energies. Our results (Fig. 4.6) demonstrate that the centrality dependence both at RHIC and LHC is well described without having the need to re-tune the free parameters ($a$, $b$ and $\hat{q}_0$). To test the validity of our formalism further, we also study the azimuthal anisotropy coefficient $\nu_2$, and provide a comparison with the experimental data at RHIC and LHC energies for four different centralities (Fig. 4.7).

To do this, we use the angle-dependent equation of $R_{AA}$ to extract the Fourier coefficient $\nu_2$ given as

$$R_{AA}(p_T, \phi) = R_{AA} \left[ 1 + 2\nu_2 \cos(2\phi - 2\psi) + \ldots \right],$$

(4.50)

where $\phi$ is the azimuthal angle and $\psi$ is the event plane angle determined by the elliptic flow
Figure 4.7: Azimuthal anisotropy $v_2$ of hadrons based on higher-twist energy-loss approach with a scale dependent $\hat{q}$ using prescription $[A]$. The QGP-PDF shown with blue dashed line in Fig. 4.10(c,d) is used as input PDF in scale evolution of $\hat{q}$. The fit parameters are fixed by the angle integrated hadron-$R_{AA}$ calculations.

of soft hadrons. We define $R_{AA}$ in-plane ($\phi \in [0, \pi/4]$) and out-plane ($\phi \in [\pi/4, \pi/2]$) as

$$R_{in} = \frac{\pi}{4} \int_{0}^{\pi/4} d\phi R_{AA}(p_T, \phi), \quad R_{out} = \int_{\pi/4}^{\pi/2} d\phi R_{AA}(p_T, \phi),$$

(4.51)

respectively. This allows us to extract $v_2$ through equation given as

$$v_2 = \frac{\pi}{4} \left[ \frac{R_{in} - R_{out}}{R_{in} + R_{out}} \right].$$

(4.52)
We do again a parameter-free calculation with the input parameters \((a, b, \hat{q}_0)\) set by the angle integrated \(R_{AA}\) calculations and show a plot of \(v_2\) (Fig. 4.7) as a function of hadron-\(p_T\) for four-different centralities at RHIC and LHC collision energies. We emphasize here that \(v_2\) results shown in Fig. 4.7 are obtained without any re-fitting of the data, i.e. all the fit parameters have been set by the \(R_{AA}\) calculations. We reproduce experimental data of \(v_2\) for hadrons with \(p_T > 10\) GeV/c at RHIC and \(p_T > 15\) GeV/c at LHC with combined \(\chi^2_{dof} = 4.0\). This is one of the attractive features of our formalism that we can describe both single-hadron observables \(R_{AA}\), and \(v_2\) with reasonable accuracy through a single framework.

Next, we follow similar methodology, but use prescription \([B]\) (Eq. 4.43); for this case the centrality dependent \(R_{AA}\) is presented in Fig. 4.8. This demonstrates the somewhat mild sensitivity to the chosen prescription for the calculation of \(\hat{q}\). In this case, the input QGP-PDF is valence-like and shown with solid lines in Fig. 4.10. For prescription \([B]\), we also show the centrality dependence of \(v_2\) at RHIC and LHC energies in Fig. 4.9. There is no re-tunning of the parameters; all the parameters are fixed in the angle-integrated \(R_{AA}\) calculations.

### 4.6 The quasi-particle distribution inside QGP in terms of PDF

In the previous section, we have demonstrated that the higher-twist energy loss formalism with scale-dependent \(\hat{q}\) gives a simultaneous description of the hadron-\(R_{AA}\) suppression at RHIC and LHC energies. For prescription \([A]\), a sea-like distribution produces the best fit, whereas for prescription \([B]\), a valence-like distribution. This indicates that the scale dependence of \(\hat{q}\) is indeed a physical effect. To explore different possible QGP-PDF that may produce similar \(\chi^2_{dof}\), we attempted several values of \(a\) and \(b\). We computed combined \(\chi^2_{dof}\) for simultaneous fits of hadron-\(R_{AA}\) at most central RHIC and LHC collisions as outlined previously.

We plot the combined \(\chi^2_{dof}\) as a function of \(a - b\) for various input PDFs. The PDF with \(a - b < 0\) corresponds to sea-like PDF, whereas \(a - b > 0\) corresponds to valence-like PDF. This allowed us to isolate the input distribution, and we show a band of input PDFs.
Figure 4.8: Nuclear modification factor $R_{AA}$ of hadrons based on higher-twist approach with a scale dependent $\hat{q}$ using prescription [B]. The QGP-PDF shown with blue solid line in Fig. 4.10(c,d) is used as input PDF in scale evolution of $\hat{q}$.

that reproduces the hadron-$R_{AA}$ data at RHIC and LHC simultaneously with a combined $\chi^2_{DOF} < 8.0$. The best-fit PDF for prescription [A] is shown in blue dashed line which give rise to combined $\chi^2_{DOF} = 4.8$ ($R_{AA}$ in Fig. 4.6). Whereas, the best-fit PDF for prescription [B] is shown in blue solid line which give rise to combined $\chi^2_{DOF} = 5.4$ ($R_{AA}$ in Fig. 4.8).

We observe that the QGP-PDF at scale $\mu^2 = 1$ GeV$^2$ has a sea-like as well as a narrow-valence like distribution. The wide bump near $x \approx 0.8$ supports the calculation for the temperature-dependent plasma with quasi-particles. The large sea contribution can be at-
Figure 4.9: Azimuthal anisotropy $v_2$ of hadrons based on higher-twist energy-loss approach with a scale dependent $\hat{q}$ using prescription [B]. The QGP-PDF shown with blue solid line in Fig. 4.10(c,d) is used as input PDF in scale evolution of $\hat{q}$. The fit parameters are fixed by the angle integrated hadron-$R_{AA}$ calculations.

Contributed to the soft particles exchanged within the interacting quasi-particle. The above calculations have been performed with choosing the rest-mass of the QGP-DOF to be $M = 1$ GeV. However, we also explored the case where $M = 2$ GeV; this choice deteriorates fits to the data, increasing the $\chi^2_{DOF} > 8$. This bolsters our assumption that the QGP-DOF with a rest-mass of 1 GeV captures the relevant degree of freedom of the plasma.
4.7 Conclusion and discussion

In this work, we have demonstrated a first successful explanation of the JET collaboration $\hat{q}$ puzzle through a scale-dependent formulation of $\hat{q}$. At a fixed temperature, enhancement of the interaction strength $\hat{q}/T^3$ at RHIC collision energies relative to LHC is mainly due to increased resolution of higher virtuality partons at higher jet energies at the LHC. As the virtuality of the hard parton increases with energy, the transverse size of the dipole formed by the hard parton and the emitted gluon decreases. As a result, the dipole can only sample gluons from the medium that have wavelengths comparable to this size. Alternatively, the exchanged transverse momentum $k_\perp^2$ has to be on the order of the transverse momentum of the emitted gluon ($l_\perp^2$) to effect medium-induced radiation (as shown in Fig. 3.2). This causes the jet parton to become sensitive to harder gluons emitted from the medium. For $k_\perp^2 > 1 \text{ GeV}^2$, we calculated this using a perturbative QCD where the hard parton exchanges single gluon with QGP-DOF.

Several approximations were made in this first attempt of scale-dependent formulation of $\hat{q}$. The energy loss calculation was derived in the regime where the hard parton carries high energy and high virtuality. In this regime, the parton shower is radiation dominant with a few scatterings in the plasma. Moreover, the multiple scatterings were considered to be independent of each other. Due to the lack of knowledge of the mass of QGP-DOF, we used estimates from finite temperature field theory and determined the upper limit of the rest-mass of QGP-DOF to be $M = 1 \text{ GeV}$. To numerically carry this out, we defined $\hat{q}(\mu^2)$ using two different prescriptions for the range of transverse momentum exchanged in the calculation of $\hat{q}$. This was performed to restrict the lower limit of the exchanged transverse momentum to always remain in the region $k_\perp^2 \geq 1 \text{ GeV}^2$. A comparison of these approximations for the resulting $\hat{q}$ as a function of the scale $\mu^2$ is presented in Fig. 4.10(b).

To further support our formalism, we also studied the Fourier coefficient $\nu_2$ which characterizes the anisotropy in the azimuthal pattern of the particle distribution. This was achieved by doing a parameter-free calculation, i.e., parameters are entirely fixed from the
angle-integrated $R_{AA}$ calculation. We successfully reproduced the experimental data at RHIC and LHC for four different centralities, without having to readjust the free parameters of our formalism. Our analysis required an input QGP-PDF at scale $\mu^2 = 1$ GeV$^2$, extracted by fitting the $R_{AA}$ data at PHENIX (0-10%) and CMS (0-5%). We performed a combined $\chi^2$ analysis to constrain the QGP-PDFs and obtain a band of uncertainty in the input distribution. The band in Fig. 4.10(c,d) provides an insight into the nature of entities inside QGP. When QGP is probed at scale $\mu^2 = 1$ GeV$^2$, the quasi-particle inside the QGP appears to have a large sea-like as well as a valence-like momentum distribution with a peak around $x \approx 0.8$.

The new formulation of $\hat{q}$ presented in this chapter provides for the first time a successful simultaneous description of haron-$R_{AA}$ data at RHIC and LHC without having the need for an arbitrary renormalization of $\hat{q}/T^3$ between RHIC and LHC. This demonstrates that scale dependence of $\hat{q}$ is a physical effect that should be accounted for in the calculation of energy loss in QGP. This analysis also constrains the momentum distribution of the quasi-particles inside the QGP.

In this chapter, the temperature dependence of $\hat{q}$ is parameterized using the local entropy density of the plasma. Also, since our scale dependent formalism of $\hat{q}$ was based on the perturbative QCD, the transport coefficient $\hat{q}$ did not include the contributions from the soft exchanges between the hard parton and the medium. In the next chapters, we would like to develop a first principle framework to evaluate the transport coefficient $\hat{q}$ using the lattice gauge theory. We shall extract the temperature dependence of $\hat{q}$ on both quenched and unquenched SU(3) lattices.
Figure 4.10: Extraction of the quasi-particle distribution inside QGP-DOF: $G_{QGP}(x, \mu^2 = 1\text{GeV}^2) = N x^a(1 - x)^b$. (a) Combined $\chi^2_{dof}$ from fits to hadron-$R_{AA}$ data at most central RHIC and LHC collision energies. The region where $a - b < 0$ corresponds to sea-like PDFs, whereas $a - b > 0$ corresponds to valence like PDFs. (b) For a fix temperature (entropy density) and an overall normalization factor, we plot $\hat{q}/T^3$ as a function of the resolution scale $\mu^2$ for three different range of $\vec{k}_\perp^2$ integration. The hard parton energy (in rest-frame of QGP-DOF) is set to be $E = 50$ GeV. The range $\vec{k}_\perp^2 \in [\mu^2/4, 9\mu^2/4]$ favors sea-like PDF, whereas $\vec{k}_\perp^2 \in [\mu^2, 9\mu^2]$ and $\vec{k}_\perp^2 \in [\mu^2, 2EM]$ favors valence-like PDF. (c) Extracted QGP-PDF at scale $\mu^2 = 1$ GeV$^2$ that gives combined $\chi^2_{DOF} < 8.0$. (c) The momentum fraction weighted PDF (same as (c)).
CHAPTER 5 REVIEW OF LATTICE QCD

In the previous chapter, we attempted to understand the scale dependence of $\hat{q}$ using the framework of perturbative QCD (pQCD). The temperature dependence of $\hat{q}$ was parameterized using the local entropy density of the plasma. Since $\hat{q}$ was formulated based on the pQCD, the transport coefficient $\hat{q}$ did not include the contributions from the soft exchanges between the hard parton and the medium. While the scale dependence seems to indicate the reason behind the enhancement of the interaction strength $\hat{q}/T^3$ at RHIC compared to LHC, we still want to look at the temperature dependence of $\hat{q}$ from first principles.

In this chapter, we present a brief review of the basic elements of lattice QCD. We shall discuss the underlying concepts in setting up actions for the gauge fields and fermion fields on the lattice. This chapter will serve as a basis for our lattice formulation of transport coefficient $\hat{q}$ to be presented in the next chapter.

5.1 Basic Elements of Lattice QCD

In this section we describe Lattice QCD [11,95–99], a tool to calculate non-perturbative observables from first principles. In the Feynman path integral formalism of quantum field theory, we define the expectation value of an observable as

$$
< O > = \frac{\int D A^a_\mu D\psi D\bar{\psi} O(A, \psi, \bar{\psi}) e^{-iS_{\text{QCD}}}}{\int D A^a_\mu D\psi D\bar{\psi} e^{-iS_{\text{QCD}}}},
$$

(5.1)

where $\psi(x)$ and $A^a_\mu(x)$ are quark field and gluon field, respectively. The exponential factor $e^{-iS_{\text{QCD}}}$ is imaginary, and hence strong oscillations for large $S_{\text{QCD}}$ makes the direct numerical computation intractable. But it is possible to perform the numerical simulation and evaluate the expectation value of an observable in the Euclidean space.

The Minkowski QCD Lagrangian is given as

$$
L_{\text{QCD}} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi + \bar{\psi}\gamma^\mu \lambda^a \frac{\gamma}{2} A^a_\mu \psi,
$$

(5.2)

where $S_{\text{QCD}} = \int d^4x L_{\text{QCD}}$, $\gamma^\mu$’s are Dirac matrices, $\lambda^a$’s are Gell-Mann matrices. To get
the Euclidean action $S_E$ from the Minkoswki QCD action, we transform 0\textsuperscript{th}-component of a Lorentz vector into an imaginary variable (also called Wick’s rotation). Thus,

$$
t \rightarrow -i \tau,
\partial_t \rightarrow i \partial_\tau,
A_0^a \rightarrow i A_4^a.
$$

This makes the exponential factor $e^{i S_{QCD}} \rightarrow e^{S_E}$ real and enables one to use it as a probability distribution function and generate ensembles of a system. Thus, in Euclidean space, we write the expectation value of an observable ($O$) as

$$
<O> = \frac{\int D A_\mu^a D \psi D \bar{\psi} O(A, \psi, \bar{\psi}) e^{-S_E}}{\int D A_\mu^a D \psi D \bar{\psi} e^{-S_E}}.
$$

We formulate Lattice QCD in Euclidean space-time with following key features \cite{11, 96, 99}

- A lattice site in a four-dimensional (4D) grid is specified by the coordinate $x_\mu = an_\mu$ where $n_\mu = (n_x, n_y, n_z, \text{and}) n_\tau$ is a 4-component vector. For calculation at finite temperature, the number of sites in the spatial directions are set to be a multiple of the number of sites in the temporal direction, whereas vacuum calculations are done with at least as many sites in the spatial directions, in our case with the same number of sites in all four directions. We denote $a$ to represent lattice spacing, i.e., the distance between neighboring lattice sites. Generally, isotropic lattices with the same lattice spacing in all directions are employed in the calculation. The fermion fields are defined on the lattice site.

- A link is defined as a directed line segment joining the nearest neighboring lattice sites with coordinate $x$ and $x + a \hat{\mu}$, where $\hat{\mu}$ is a unit vector along the direction of $\mu$. The purpose of introducing links on the lattice is that we define the gauge field on it by attaching a $SU(N)$ matrix, also called a link variable (Fig. 5.1) denoted as $U_\mu(x)$. The
link in the reverse direction $U_{-\mu}(x + a\hat{\mu})$ is given by the Hermitian conjugate of the link variable $U_\mu(x)$. If $g(x)$ is an element of the gauge group of $SU(N)$ theory, then the link variable should have the following transformation property:

$$U_\mu(x) \rightarrow U'_\mu(x) = g(x)U_\mu(x)g^\dagger(x + a\hat{\mu}).$$

A link variable $U_\mu(x)$ is related to the continuum gluon field by

$$U_\mu(x) = Pe^{ig_0 \int_x^{x + a\hat{\mu}} A_\mu(x)dx},$$

where $A_\mu(x) = \sum_{i=1}^{8} t^a A^a_\mu(x)$ with $t^a = \lambda^a/2$ and $\lambda^a$ are the Gell-Mann matrices. The symbol $P$ refers to path-ordering for the non-commuting matrices $A_\mu(x)$.

Lattice calculation requires a way to compute the Euclidean action $S$. To compute this we employ a concept of a plaquette which is an elementary square bounded by four links as shown in Fig. 5.2. We associate with this square loop a quantity called plaquette variable given as

$$U_{\mu,\nu}(x) = U_\mu(x)U_\nu(x + a\hat{\mu})U^\dagger_\mu(x + a\hat{\nu})U^\dagger_\nu(x).$$

The usefulness of $U_{\mu,\nu}$ is that it can be used to construct an action. The trace of $U_{\mu,\nu}$ is a gauge invariant quantity (see invariance by applying transformation given in Eq. 5.5). Using Baker-Campbell-Hausdorff identity

$$e^{A+B} = e^{(A+B+\frac{1}{2}[A,B]+...)} ,$$

and Eq. 5.6 and performing the Taylor expansion of the gauge field around $x$, we
simplify $U_{\mu,\nu}$ given in Eq. 5.7 to get

$$\text{Tr}(F_{\mu\nu}^2) = \lim_{a \to 0} \frac{2N_c}{g_0^2 a^4} \left[ 1 - \frac{\text{Re}(\text{Tr}[U_{\mu,\nu}])}{N_c} \right] + \mathcal{O}(a^2). \quad (5.9)$$

Thus, quantum mechanical action for $SU(N)$ should be

$$S = \int \text{Tr}\left[ \frac{1}{2} F_{\mu\nu} F^{\mu\nu} \right] d^4x$$

$$= \lim_{a \to 0} \sum_{x,\mu<\nu} \frac{2N_c}{g_0^2} \left[ 1 - \frac{\text{Re}(\text{Tr}[U_{\mu,\nu}(x)])}{N} \right]. \quad (5.10)$$

• To generate $SU(N)$ gauge field configurations we require objects called staple. A staple is a path-ordered product of the three gauge link variables that build up the plaquette around a given link in a given plane as shown in Fig. 5.3. For a given link, we will have six such staples, with two staples in each of the three planes. Note, the sum of staples is not a $SU(N)$ matrix.

Figure 5.1: Gauge field are defined through link variable $U_\mu(x)$. Hermitian conjugate of $U_\mu(x)$ represents link in the opposite direction. Lattice spacing is $a$. [11]

• The partition function in lattice gauge theory can be written in terms of the link variable and fermion field as

$$Z(\beta) = \int \prod_{x,\mu} dU_\mu(x) \prod_x [d\bar{\psi}_x d\psi_x] e^{-S_G - S_F} \quad (5.11)$$

where $S_G$ is the pure gauge action, $S_F$ is fermion action, $\beta$ is inverse temperature, $dU_\mu(x)$ indicate integration over link variables and $d\bar{\psi}_x d\psi_x$ indicate integration over
the fermion fields. In analytic calculations, fermions are represented by the Grassmann variables $\psi_x$ and $\bar{\psi}_x$ due to which it is not possible to directly assign them on the lattice.
A generic fermion action can be written as

\[ S_F = a^4 \sum_{x,y} \bar{\psi}_x (\not \! D + m)_{F;x,y} \psi_y, \]  

(5.12)

where \((\not \! D + m)_{F;x,y}\) is a lattice discretization of the continuum Dirac operator \(\not \! D + m\). The subtleties involved in setting up fermions on the lattice will be discussed in the later sections. Since, the action \(S_F\) is quadratic in the fermion fields, the integrations over the Grassmann variables can be carried out to get following expression,

\[ Z(\beta) = \int \prod_{x,\mu} dU_\mu(x) \det(\not \! D + m) e^{-S_G}, \]  

(5.13)

where \(\beta\) is inverse of temperature.

Thus, the expectation value of any observable \(O\) can be written as

\[ \langle O \rangle = \frac{1}{Z(\beta)} \int \prod_{x,\mu} dU_\mu(x) \, O \det(\not \! D + m) \, e^{-S_G} \]  

(5.14)

In Eq. 5.14 it is assumed that the observable \(O\) does not involve fermion fields \(\psi_x\) and \(\bar{\psi}_x\). However, in the cases where observable do involves \(\psi_x\) and \(\bar{\psi}_x\), then one needs to perform Wick’s contractions and each pair is replaced by \((\not \! D + m)^{-1}_{F;x,y}\). The calculations performed on the lattice without accounting for the sea quarks are called quenched calculations and one sets \(\det(\not \! D + m) = 1\). Note, we will reserve the parameter \(\beta\) for temperature, whereas we shall use \(\beta_0\) to represent the bare coupling factor \(2N_c/g^2\) or \(10/g^2\).

5.2 Generating gauge field configuration

In this section, we review algorithms to generate \(SU(2)\) and \(SU(3)\) gauge field configurations on the lattice \[97\, 100\, 103\]. This is done by initializing gauge links to an ordered or random set of \(SU(N)\) matrices and then successively bringing them into contact with a heat bath. Each link variable is replaced by a new link variable chosen based on a probability distribution, keeping all the other links fixed at their previous values. This local updating...
only applies to the pure gauge cases. For Full QCD, the quark determinant does not permit local updating. A hybrid Monte Carlo algorithm (HMC) is needed for global updating [104].

5.2.1 SU(2) gauge field

First, we discuss an algorithm for SU(2) gauge field. We know that $SU(2)$ group requires 3 independent parameters to fully specify its group elements. Thus, we can parametrize it in the following form:

$$U = a_0 I + i \vec{a} \cdot \vec{\sigma},$$

(5.15)

where $a_0, \vec{a}$ are real numbers satisfying condition $a_0^2 + \vec{a}^2 = 1$, and $\sigma_i$ represents well-known Pauli matrices. We generate $SU(2)$ matrix defined on gauge links with the following probability distribution:

$$dP[U] \propto dU \ e^{-S[U]}.$$  

(5.16)

While working on a given link, we only need to consider the contribution to the action coming from the six plaquettes containing that link. Using the above equations and by defining staples as $\tilde{U}_{n=1,\ldots,6}$, we can simplify the probability distribution to

$$dP[U] \propto \exp \left( -\beta_0 \sum \left( 1 - \frac{\text{Re Tr}(U_{\mu \nu})}{N} \right) \right) dU.$$  

(5.17)

Using the fact that addition of the two $SU(2)$ matrix is proportional to $SU(2)$ matrix, one can simplify the equation as follows:

$$\sum_{n=1}^{6} \tilde{U}_n = k \bar{U},$$  

(5.18)

where $\bar{U}$ is a $SU(2)$ matrix, $k$ is an unknown constant to be determined. We determine $k$
by taking determinant on both the side of the above equation, i.e.
\[
\det \left( \sum_{n=1}^{6} \tilde{U}_n \right) = \det(k\tilde{U}) = k^2
\]

\[\implies k = \left( \det \left( \sum_{n=1}^{6} \tilde{U}_n \right) \right)^{\frac{1}{2}}.\]

Thus, the probability distribution becomes
\[
dP(U\tilde{U}^{-1}) \propto \exp \left( \frac{\beta_0 k}{N} \text{Re} \text{Tr}(U) \right) dU.
\] (5.20)

Now, we insert the invariant group measure and the trace of the link variable $U$ i.e. $\text{Tr}(U) = \text{Tr}(a_0 + i\vec{a}\vec{\sigma}) = 2a_0$ to get
\[
dP(U\tilde{U}^{-1}) \propto \frac{\delta(a_0^2 + |\vec{a}|^2 - 1)}{2\pi^2} \exp \left( \frac{2\beta_0 k}{N}a_0 \right) d^4a
\]
\[
\propto |\vec{a}| \exp \left( \frac{2\beta_0 k}{N}a_0 \right) da_0 d\Omega,
\] (5.21)

where $d\Omega$ is the differential solid angle of $\vec{a} = \sqrt{a_1^2 + a_2^2 + a_3^2}$.

So, we will need to sample $a_0$ in range $[-1, 1]$ with probability:
\[
P(a_0) \propto \left( \sqrt{1 - a_0^2} \right) \exp \left( \frac{2\beta_0 k}{N}a_0 \right).
\] (5.22)

The vector $\vec{a}$ is generate by generating azimuthal angle $\phi$ and $\cos(\theta)$ randomly in range $[0, 2\pi]$ and range $[-1, 1]$, respectively. Given the matrix $U$ generated using the above procedure, the new link variable on the lattice is given by $U' = U\tilde{U}^{-1}$.

5.2.2 $SU(3)$ gauge field

In this section, we describe a method of generating and updating color $SU(3)$ matrix $U_\mu(x)$ defined as gauge links on a lattice $\Box$. The $SU(3)$ matrix of the gauge links should
be generated using the following probability distribution:

$$dP[U] \propto dU e^{-S[U]}.$$  \hfill \text{(5.23)}

Since, $SU(3)$ group has 8 independent parameters, it is tedious to generate $SU(3)$ matrix with above probability distribution directly.

We employ a concept of subgroup to simplify the problem. To cover $SU(3)$ group fully, one needs 3 different $SU(2)$ groups. Since, $SU(3)$ is composed of 3x3 matrix, we choose $SU(2)$ matrix of form:

$$\begin{align*}
A_1 &= \begin{bmatrix} a_{111} & a_{112} & 0 \\ a_{121} & a_{122} & 0 \\ 0 & 0 & 1 \end{bmatrix} ;
A_2 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & a_{222} & a_{223} \\ 0 & a_{232} & a_{233} \end{bmatrix} ;
A_3 &= \begin{bmatrix} a_{311} & 0 & a_{313} \\ 0 & 1 & 0 \\ a_{331} & 0 & a_{333} \end{bmatrix} ,
\end{align*}$$

where $a_1, a_2, a_3 \in SU(2)$. In each step of iteration a new link variable ($U_{new}$) is obtained by multiplying the old link ($U_{old}$) by three newly generated $SU(3)$ matrix $A_1, A_2$ and $A_3$, i.e.

$$U_{new} = A_3 * A_2 * A_1 * U_{old}.$$  \hfill \text{(5.25)}

$A_k$’s are generated using following probability distribution $dP[A_k] \propto dA_k e^{-S[A_k]}$.

We represent action $S$ in terms of Wilson action:

$$dP[A_k] \propto dA_k \ e^{-\frac{\beta}{N} \Re(\text{Tr}(A_k U^{(k-1)} \tilde{U}_\Box))},$$

where $U^{(k-1)} = A_{k-1} \ldots A_1 U_{old}$, $U^0 = U_{old}$, and $\tilde{U}_\Box$ represents summation over six staples shown in Fig. 5.3. We define $R_k = U^{(k-1)} \tilde{U}_\Box$. Since $A_k$ is a block matrix, we can write

$$\Re(\text{Tr}(A_k U^{(k-1)} \tilde{U}_\Box)) = \Re(\text{Tr}(a_k * r_k)) + \text{terms independent of } (a_k)_{ij},$$

\hfill \text{(5.27)}
where \( r_k \) is a submatrix of \( R_k \) with same block structure as \( A_k \). Thus, the probability distribution becomes

\[
dP[a_k] \propto da_k \ e^{-\frac{\beta_0}{N} \text{Re}(\text{Tr}(a_k r_k))}.
\]  
(5.28)

Note that \( r_k \) is a 2x2 matrix which does not need be a \( SU(2) \) matrix. We can further simplify the above equation by writing:

\[
r_k = r_0 I + i \vec{r}.\vec{\sigma}, \quad a_k = \alpha_0 I + i \vec{\alpha}.\vec{\sigma},
\]  
(5.29)

where \( r_0 \) and \( \vec{r} \) are complex numbers. Thus, we have

\[
\text{Re}(\text{Tr}(a_k r_k)) = 2(\alpha_0 \text{Re}(r_0)) - \vec{\alpha}.\text{Re}(\vec{r}).
\]  
(5.30)

Now, the probability distribution reduces to

\[
dP[\alpha_k] \propto d^4 \alpha_k \delta(\alpha^2 - 1) e^{-\frac{\beta_0}{N} \text{Re}(\text{Tr}(a_k r_k))},
\]  
(5.31)

which is similar to the distribution given in Eq. (5.21). Thus, we generate \( \alpha_k \)'s with the above probability distribution using the algorithm described in subsection 5.2.1.

5.3 Lattice actions

In this section, we briefly review a few popular actions used in lattice QCD.

5.3.1 Wilson’s gauge action

The study of lattice QCD essentially started from Wilson’s formulation of the gauge theory that employed a gauge invariant plaquette action \[95\] built using the four-link square closed loops. This action is now known as Wilson’s gauge action and given as

\[
S_{G_{\text{Wilson}}} = \beta_0 \sum_{x,\mu<\nu} \left[ 1 - \frac{1}{N_c} \text{Re}(\text{Tr}[U_{\mu,\nu}(x)]) \right]
\rightarrow a^4 \sum_x \left[ \frac{1}{4} F_{\mu \nu}^a(x) F_{\mu \nu}^a(x) + O(a^2) \right],
\]  
(5.32)
where $U_{\mu,\nu}(x)$ is the plaquette operator defined in Eq. 5.7. The $\beta_0$ is given by

$$\beta_0 = \frac{2N_c}{g_0^2}. \tag{5.33}$$

The leading discretization errors in Wilson’s action is on the order of $O(a^2)$.

### 5.3.2 Tree-level Symanzik’s improved gauge action

In the Symanzik approach \cite{105,106}, in addition to the four-link plaquette, one adds the planar six-link rectangular closed loops. The product (path-ordered) of links on the $2 \times 1$ or $1 \times 2$ rectangular closed loop can written as

$$R_{\mu,\nu}(x) = U_{\mu}(x)U_{\mu}(x + a\hat{\mu})U_{\nu}(x + 2a\hat{\mu})U_{\mu}^\dagger(x + a\hat{\mu} + a\hat{\nu})U_{\mu}^\dagger(x + a\hat{\nu})U_{\nu}(x); \ \mu \neq \nu. \tag{5.34}$$

Adding the rectangle and square loops contributions, we get

$$S^\text{Imp}_G = \beta_0 \left[ \sum_{x, \mu \neq \nu} \left[ 1 - \frac{1}{3} \text{ReTr}(U_{\mu,\nu}(x)) \right] - \frac{1}{20} \sum_{x, \mu \neq \nu} \left[ 1 - \frac{1}{3} \text{ReTr}(R_{\mu,\nu}(x)) \right] \right]$$

$$\rightarrow a^4 \sum_x \left[ \frac{1}{4} F^{a}_{\mu\nu}(x) F^{a}_{\mu\nu}(x) + O(a^4) + O(g_0^2 a^2) \right]. \tag{5.35}$$

In this case, the input parameter $\beta_0$ is given by

$$\beta_0 = \frac{10}{g_0^2}. \tag{5.36}$$

In Symanzik gauge improvement program, the coefficients of the gauge action are chosen to improve the discretization error by removing the leading corrections order-by-order in perturbation theory. The tree-level discretization errors in the action (Eq. 5.35) is on the order of $O(a^4)$ and $O(g_0^2 a^2)$. We shall employ the tree-level Symanzik’s gauge action in the study of the unquenched lattices.
5.3.3 Naive quark action

Finding a good fermion action on the lattice is much more difficult compared to the
gauge action. Naively, one can discretize the derivative in the fermion action using leap-frog
method as

$$\partial_\mu \psi(x) \to \frac{1}{2a} \left[ \psi(x + a \hat{\mu}) - \psi(x - a \hat{\mu}) \right]$$

(5.37)

Using this, the naive quark action can be written as

$$S_{\text{naive}} = a^4 \sum_{x, \mu} \frac{1}{2a} \left[ \bar{\psi}(x) \gamma^\mu \{ U_\mu(x) \psi(x + a \hat{\mu}) - U_\mu^\dagger(x - a \hat{\mu}) \psi(x - a \hat{\mu}) \} \right] + a^4 \sum_x m_f \bar{\psi}(x) \psi(x).$$

(5.38)

One can check that the above discretization of the fermion action is invariant under gauge
transformations: $\psi(x) \to g(x) \psi(x)$ and $\bar{\psi}(x) \to \bar{\psi}(x) g^\dagger(x)$. However, when it comes to
physical interpretation of the quark propagator, a few severe problems are identified.

The free propagator for above discretization of the fermion action can be written as

$$G_{\text{naive}}(x, y) = \langle \bar{\psi}(x) \psi(y) \rangle = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} \frac{m_f - \frac{i}{a} \sum_\mu \gamma^\mu \sin(p_\mu a)}{m_f^2 + \frac{1}{a^2} \sum_\mu \sin^2(p_\mu a)} e^{ip(x-y)}.$$ 

(5.39)

In the massless limit, the above Eq. 5.39 shows that there are poles at momentum $p_\mu = \pi/a$,
where, $\mu = 1, 2, 3$ and 4. Moreover, this indicates that there are $2^4$ distinct poles although we
started with a single free fermion in the action. Thus, the naive discretization of the quark
action gives rise to 15 additional degrees of freedom that are unphysical. This behaviour is
referred to as fermion doubling problem and the additional degrees of freedom are referred to as
“taste” (unphysical flavor) of the quark. This unusual appearance of “tastes” of quarks have
surprising consequences. For instance, the standard low-energy quark can absorbs a virtual
gluon such that it is not driven off energy-shell, and then turn into a quark of another taste.

In quark-quark scattering, the dominant flavor-changing interaction is one-gluon exchange
5.3.4 Staggered quark action

Staggered quark discretization was first proposed by Kogut and Sussking (Ref. [107,108]) to circumvent the problem of fermion doubling in the naive quark action. In this method, one diagonalize $\gamma$ matrices in the naive fermion action by transforming the fermion fields as

$$\psi(x) \rightarrow \Gamma(x)\psi(x); \quad \bar{\psi}(x) \rightarrow \bar{\psi}(x)\Gamma^\dagger(x)$$

(5.40)

The popular choice for $\Gamma(x)$ is

$$\Gamma(x) = \gamma_1^{(x_1/a)}\gamma_2^{(x_2/a)}\gamma_3^{(x_3/a)}\gamma_4^{(x_4/a)}; \quad x_\mu = n_\mu a; \quad \text{where, } n_\mu \in \mathbb{Z}.$$  

(5.41)

Here,

$$\eta_\mu(x) = (-1)^{(x_1+1)\cdots+x_{\mu-1}}(x_1+1)\cdots+x_{\mu-1})/a$$

(5.42)

Applying the above transformation, we arrive at the staggered quark (SQ) action

$$S_{SQ}^F = a^4 \sum_{x,\mu} \frac{1}{2a} \eta_\mu(x)\bar{\psi}(x) \left[ U_\mu(x)\psi(x + a\hat{\mu}) - U_\mu^\dagger(x - a\hat{\mu})\psi(x - a\hat{\mu}) \right] + a^4 \sum_x m_f \bar{\psi}(x)\psi(x)$$

(5.43)

In the above equation, due to the diagonalization of $\gamma$ matrices, the spinor components of $\psi(x)$ can be completely decoupled from each other. Then, the three out of the four components can be dropped and the action is re-written in terms of the one-component spinor $\chi(x)

$$S_{SQ}^F = a^4 \sum_{x,\mu} \frac{1}{2a} \eta_\mu(x)\bar{\chi}(x) \left[ U_\mu(x)\chi(x + a\hat{\mu}) - U_\mu^\dagger(x - a\hat{\mu})\chi(x - a\hat{\mu}) \right] + a^4 \sum_x m_f \bar{\chi}(x)\chi(x)$$

(5.44)

The above staggered quark action reduces the total number of unphysical "taste" (flavors) of quarks from 16 to 4. At this point, a more popular technique, called "rooting" trick [109,110] is employed to remove the remaining unphysical flavors of quarks. In this trick, a
fourth-root of the $\det(\hat{D}_{SQ} + m_f)$ is taken, where the label $SQ$ means staggered quark. This “rooting” procedure is theoretically not well-established, but numerical results in the past seem to support the validity of this procedure $^{111,115}$.

### 5.3.5 Highly-improved staggered quark (HISQ) action

Earlier studies done on the staggered quark action with the link smearing $^{116}$ showed that the resulting action reduces the taste-changing interactions. It was first systematically demonstrated by Lepage $^{117}$ that the link smearing could be incorporated into the Symanzik improvement program. In this approach, the coefficients are computed in perturbation theory to suppress the taste violating terms order-by-order in lattice spacing $a$. The simplest smearing is obtained by replacing the link variable in the staggered quark action by adding a contribution from three-link staple-like terms:

$$U_\mu(x) \rightarrow U^{\text{fat},3}_\mu(x) = c_1 U_\mu(x) + c_3 \sum_{\nu \neq \mu} \frac{1}{2} \left[ U_\nu(x) U_\mu(x + a \hat{\nu}) U^\dagger_\nu(x + a \hat{\mu}) + U^\dagger_\nu(x - a \hat{\nu}) U_\mu(x - a \hat{\nu}) U_\nu(x + a \hat{\mu} - a \hat{\nu}) \right],$$  \hspace{1cm} (5.45)

where $U^{\text{fat},3}_\mu$ refers to the fat-link which contains the three-link staple terms. The coefficients $c_1$ and $c_3$ satisfy $c_1 + 6c_3 = 1$ due to normalization in the continuum limit. The coefficients $c_1$ and $c_3$ are chosen to minimize the taste violating terms in the action $^{118}$.

The highly improved staggered quark (HISQ) action was introduced by the HPQCD/UKQCD collaboration in Ref. $^{119}$. In this “HISQ” discretization of the quark action is written as

$$S_F^{\text{HISQ}} = a^4 \sum_{x,\mu} \eta_\mu(x) \bar{\chi}(x) \left[ \mathcal{D}_\mu^{\text{HISQ}} \right] \chi(x) + a^4 \sum_x m_f \bar{\chi}(x) \chi(x),$$  \hspace{1cm} (5.46)

where

$$\mathcal{D}_\mu^{\text{HISQ}} \equiv \Delta_\mu(W) - \frac{a^2}{6} (1 + \epsilon) \Delta^3_\mu(X),$$  \hspace{1cm} (5.47)

while $\epsilon \neq 0$ can be used to cancel quark mass corrections in the dispersion relation for heavy quarks.
The operator $\Delta_\mu$ in Eq. (5.47) refers to a discrete version of the covariant derivative,

$$\Delta_\mu(V)\chi(x) = \frac{1}{2a} \left[V_\mu(x)\chi(x + a\hat{\mu}) - V_\mu^\dagger(x - a\hat{\mu})\chi(x - a\hat{\mu})\right].$$

(5.48)

When the operators $W$ and $X$ in Eq. (5.47) are the link $U_\mu$, the resultant action is referred to as “Naik-action” [120]. However, in HISQ, the first difference operator is given as

$$W_\mu(x) = F^\text{HISQ}_\mu U_\mu(x),$$

(5.49)

where $F^\text{HISQ}_\mu$ is a doubly smeared operator. It is given as

$$F^\text{HISQ}_\mu = \left(F_\mu - \sum_{\rho \neq \mu} \frac{\alpha^2[\delta_\rho]^2}{2}\right) U F_\mu,$$

(5.50)

where operator $U$ is a re-unitarization operator and is used to reunitarize whatever it acts on.

In Eq. (5.50) operator $\delta_\rho$ approximates the first order covariant derivative given as

$$\delta_\rho U_\mu(x) = \frac{1}{a} \left[U_\rho(x)U_\mu(x + a\hat{\rho})U_\rho^\dagger(x + a\hat{\mu}) - U_\rho^\dagger(x - a\hat{\rho})U_\mu(x - a\hat{\rho})U_\rho(x + a\hat{\mu} - a\hat{\rho})\right].$$

(5.51)

The smearing operator $F_\mu$ is given as

$$F_\mu = \prod_{\rho \neq \mu} \left(1 + \frac{\alpha^2\delta_\rho^{(2)}}{4}\right),$$

(5.52)

where $\delta_\rho^{(2)}$ approximates the second-order covariant derivative given as

$$\delta_\rho^{(2)} U_\mu(x) = \frac{1}{a^2} \left[U_\rho(x)U_\mu(x + a\hat{\rho})U_\rho^\dagger(x + a\hat{\mu}) - 2U_\mu(x)
+ U_\rho^\dagger(x - a\hat{\rho})U_\mu(x - a\hat{\rho})U_\rho(x + a\hat{\mu} - a\hat{\rho})\right].$$

(5.53)
The second difference operator $X_\mu$ in HISQ (Eq. 5.47) is given as

$$X_\mu(x) = U F_\mu U_\mu(x). \quad (5.54)$$

Among the currently used staggered fermion actions [41,42], the HISQ action is known to yield the smallest violations of taste-changing interactions and removes all tree-level $O(a^2)$ errors in the naive quark actions.

### 5.4 Monte Carlo averages and Jackknife error analysis

The final step in Monte Carlo is performing statistical analysis of the measured observables and accounting for sources of error. For a given set of $N$ number of gauge configurations, the expectation value of an operator $O$ can be written as

$$\bar{O} = \langle O(U) \rangle = \frac{1}{N} \sum_{i=1}^{N} O_i(U) + O\left(\frac{1}{\sqrt{N}}\right), \quad (5.55)$$

In cases where all the gauge configurations are independent, the statistical error is given by the standard definition of variance:

$$\sigma_{\text{naive}} = \sqrt{\frac{\sum_{i=1}^{N} [\bar{O} - O_i(U)]^2}{N(N-1)}} \quad (5.56)$$

But, in our case, the generated gauge configurations are the result of a (compute-)time series in Monte Carlo simulation in which the successive configurations are correlated.

One of the popular ways to estimate the auto-correlation of the data is to use apply “Data blocking” method and use the block results to compute the mean and variance using “Jackknife” method [99]. In data blocking method, we divide the data $\{x_1, x_2, \ldots, x_N\}$ into sub-blocks of data with size $N$, and compute the block mean values $X_1, X_2, \ldots, X_N$. Now, we use the resultant data to compute the mean and error. In jackknife method, we construct $N$ subsets by removing the $i^{th}$ entry from the data set $\{X_1, X_2, \ldots, X_N\}$ and determine the
mean value $X_i^J$ for each set. The jackknife average is given as

$$\bar{X}^J = \frac{1}{N} \sum_{i=1}^{N} X_i^J. \quad (5.57)$$

Then, the standard deviation in the mean is calculated by

$$\sigma_{X^J} = \sqrt{\frac{N-1}{N} \sum_{i=1}^{N} [X_i^J - \bar{X}^J]^2} \quad (5.58)$$

Often, in real calculation, one is interested in computing a quantity that are usually functions of two or more observables. To propagate the error in this scenario, we give an example by considering a function $f(x,y)$ that depends on two observables $x$ and $y$. Let’s assume \{X_1, X_2, ..., X_N\} and \{Y_1, Y_2, ..., Y_N\} the data set represents a block average for observables $x$ and $y$, respectively. The jackknife average is given by

$$X_i^J = \frac{1}{N-1} \sum_{j \neq i} X_j; \quad Y_i^J = \frac{1}{N-1} \sum_{j \neq i} Y_j; \quad (5.59)$$

Then, the jackknife mean of function $f(x,y)$ is given by

$$\bar{f} = \langle f(x,y) \rangle = \frac{1}{N} \sum_{i=1}^{N} f(X_i^J, Y_i^J). \quad (5.60)$$

The jackknife error in $\bar{f}$ is given by

$$\sigma_J = \sqrt{\frac{N-1}{N} \sum_{i=1}^{N} [f(X_i^J, Y_i^J) - \bar{f}]^2}. \quad (5.61)$$
CHAPTER 6  LATTICE DETERMINATION OF TRANSPORT COEFFICIENT $\hat{q}$

Over the past decades, the phenomenon of jet quenching has been well established as an indicator of the formation of the quark-gluon plasma (QGP) in heavy-ion collisions. Among existing known coefficients characterizing transport properties of the hard parton traversing QGP, the jet transport coefficient $\hat{q}$ is the leading transport coefficient that controls the modification of jets inside the QGP. It introduces momentum transverse to the hard parton’s direction, changing its virtuality and thus, controls the modification of hard jets in the QGP. The transport coefficient $\hat{q}$ is defined as average squared transverse momentum broadening per unit length of the medium.

Previously, several methods to compute $\hat{q}$ from first principles have been attempted, each with its own assumptions, limitations, and region of validity [12,121–131]. A finite-temperature calculation based on Hard Thermal Loop (HTL) predicts $\hat{q}$ to scale as a product of $T^3$ times log($E/T$) [125]. A lattice gauge theory based approach has also been put forward by one of the authors [12] to compute $\hat{q}$ on a 4D quenched SU(2) plasma. A well known state-of-the-art phenomenological extraction of $\hat{q}$ has come from the work by the JET collaboration [9]. This extraction is based on fits to the experimental data for the nuclear modification factor $R_{AA}$ of leading hadrons in central collisions at the Relativistic Heavy-Ion Collider (RHIC) and the Large Hadron Collider (LHC). Beyond this, it is possible that $\hat{q}$ possesses a dependence on the resolution scale of the hard parton [40,132].

In chapter 4, we presented a new formulation of $\hat{q}$ based on PDF of QGP-DOF and showed for the first time a successful simultaneous description of hadron-$R_{AA}$ data at RHIC and LHC that does not require an arbitrary normalization of $\hat{q}/T^3$ between RHIC and LHC. In that formulation, the temperature dependence of $\hat{q}$ was parameterized using the local entropy density of the plasma. In this chapter, we shall develop a first principle framework to compute the temperature dependence of the transport coefficient $\hat{q}$. We shall follow the methodology described in the article [12] and outline a method to compute $\hat{q}$ using lattice
gauge theory applicable to both the hot quark-gluon plasma and pure gluon plasma.

6.1 *Ab-initio* approach to evaluate ̂q

The transport parameter ̂q essentially measures the transverse scattering experienced by a projectile passing through the plasma. A framework to evaluate ̂q from first principles using lattice gauge theory was first proposed in Ref. [12]. In this section, we briefly discuss the *ab-initio* formulation of ̂q. Consider the propagation of a hard virtual quark with light-cone momentum \( q = (\mu^2/2q^-, q^-, 0_{\perp}) \sim (\lambda^2, 1, 0)q^- \) through a section of the plasma at temperature \( T \), where, \( \lambda \ll 1, q^- \gg \Lambda_{\text{QCD}} \), and \( \mu \) is off-shellness of the hard quark. We consider a leading order (LO) process of the hard quark traveling along the negative z-direction, exchanging a transverse gluon with the plasma. In this frame \( q^0 > 0, q_z < 0, \) and \( q^0 \leq |q_z| \). Thus, the light-cone momentum of the quark \( q^+ = \sqrt{q^0 + q^-} \leq 0 \) and \( q^- = \sqrt{q^0 - q^z} \geq 0 \).

We consider this process in the rest frame of the medium with the momentum of the exchanged gluon as \( k = (k^+, k^-, k_{\perp}) \sim (\lambda^2, \lambda^2, \lambda)q^- \). We show a LO order scattering process of the hard quark off from the medium in Fig. 6.1(a) and show the forward scattering diagram for this process in Fig. 6.1(b). We can write the scattering amplitude of the

![Diagram](image-url)

*Figure 6.1: (a) A section of the plasma at temperature \( T \). (b) Forward scattering diagram of the process shown in the figure (a) on the left.*
forward scattering diagram shown in Fig. 6.1(b) as

\[ \mathcal{M}(k) = g^2 \langle q^-; n | \int d^4x d^4y \bar{\psi}(y) A(y) \psi(y) \times \bar{\psi}(x) A(x) \psi(x) | q^-; n \rangle, \tag{6.1} \]

where \(|n\rangle\) is a thermal state with energy \(E_n\) of the medium. Using above, we can write spin-color-averaged transition probability as

\[ W(k) = \text{Disc} \frac{g^2}{2\pi i} \left[ \frac{1}{V_{N_c}} \int d^4x d^4y \langle M| \Tr \left[ \frac{q}{2E_q} A(x) \frac{(q + k)}{(q + k)^2} A(y) \right] | M \rangle \right] e^{-ik(x-y)}, \tag{6.2} \]

where \(g = \sqrt{4\pi\alpha_s}\) is the strong coupling constant at vertex of the hard quark and transverse gluon. The discontinuity in the above expression is calculated using Cutkosky’s rule and given as \(\text{Disc}[1/(q + k)^2] = -2\pi i \delta[(q + k)^2]\).

In Eq. 6.2 \(\langle M| .. |M \rangle\) represents the average over all possible initial states of the thermalized medium, weighted by a Boltzman factor, given as

\[ \langle M| .. |M \rangle = \sum_n e^{-\beta E_n} \left\langle n| .. |n \right\rangle, \tag{6.3} \]

where \(|n\rangle\) is a thermal state with energy \(E_n\) of the medium, \(\beta\) is inverse temperature and \(Z\) is the partition function of the medium without the incoming quark. To compute \(\hat{q}\), we use following form

\[ \hat{q} = \sum_k k_{\perp}^2 \frac{W(k)}{t}, \tag{6.4} \]

where \(k\) is the momentum of the exchanged gluon and \(t\) is the time spent by the hard quark in the thermal volume \(V\).

Applying standard pQCD techniques and evaluating the above expression, one obtains
the following expression for $\hat{q}$,

$$
\hat{q} = \frac{\langle \vec{k}^2 \rangle}{t} = \frac{8\sqrt{2\pi\alpha_s}}{N_c} \int \frac{dy^2 \eta^2}{(2\pi)^3} d^2k e^{-\frac{k^2}{2\eta^2}y^2 + i\vec{k}_\perp \cdot \vec{y}_\perp} \sum_n \langle n | \frac{e^{-\beta E_n}}{Z} \text{Tr}[F^{+\perp\mu}(0)F^{+\perp}_{\perp\mu}(y^-, y_\perp)] | n \rangle,
$$

(6.5)

where $t$ is the time spent by the hard quark, $F^{\mu\nu} = t^a F^{a\mu\nu}$ is the gauge field strength, $\alpha_s$ is the strong coupling constant, $\beta$ is the inverse temperature, $|n\rangle$ is a thermal state with energy $E_n$, $Z$ is the partition function of the thermal medium, and $N_c$ is the number of colors. Computing the thermal expectation value of the operator $F^{+\perp\mu}(0)F^{+\perp}_{\perp\mu}(y^-, y_\perp)$ is challenging due to the light-cone separation of the two operators.

The equation above is not gauge invariant, but is gauge covariant. To construct a gauge invariant $\hat{q}$, one needs to introduce Wilson lines. As outline in Ref. [126] one requires two Wilson lines: one along the light-cone $y^-$ direction and the other along the transverse direction $y_\perp$. A gauge invariant expression for $\hat{q}$ is given as,

$$
\hat{q} = \frac{8\sqrt{2\pi\alpha_s}}{N_c} \int \frac{dy^2 \eta^2}{(2\pi)^3} d^2k e^{-\frac{k^2}{2\eta^2}y^2 + i\vec{k}_\perp \cdot \vec{y}_\perp} \sum_n \langle n | \frac{e^{-\beta E_n}}{Z} \text{Tr}[F^{+\perp\mu}(y^-, y_\perp)U(\infty^-, y_\perp; 0^-, y_\perp)]
\times T^+(\infty^-, \infty_\perp; \infty^-, y_\perp)T(\infty^-, \infty_\perp; \infty^-, 0_\perp)U(\infty^-, 0_\perp; 0^-, 0_\perp)F^{+\perp\mu}_{\perp\mu}(0) | n \rangle,
$$

(6.6)

where $U$ represents a Wilson line along the $y^-$ light-cone direction and $T$ represents a Wilson line along the $y_\perp$ transverse light-cone direction. In light-cone gauge, $A^{a+} = 0$, only the transverse Wilson lines contribute, whereas in the covariant gauge, the only light-cone $y^-$ Wilson lines contribute. Issues related in analytic continuation of real-time separated operator to an euclidean operator, and due to infinite extent of the Wilson lines, it is extremely challenging to directly evaluate these operators on the finite size lattices.

In this study we will ignore the Wilson lines and use a method of dispersion relation to express $\hat{q}$ in terms of an infinite series of local operators that are suppressed by the powers
of the hard scale $Q^2$. Thus, $\hat{q}$ will be obtained as a series of local operators given as

$$\hat{q} = \sum_n \frac{c_n}{[Q^2]^n} O_n,$$

(6.7)

where $O_n$’s are non-perturbative local operator characterising purely the medium effects, $c_n$’s are perturbative coefficients encoding the hard quark interaction with the transverse gluon in the medium. This does not mean that the coupling within the medium is perturbatively weak. The evaluation of perturbative coefficients $c_n$, requires one to specify the gauge. Each choice of the gauge in perturbation theory will lead to a slightly different set of local operators $O_n$ and perturbative coefficients $c_n$, but the total sum will be gauge invariant.

To obtain the expression of $\hat{q}$ as a series of local operators, we define a generalized coefficient as

$$\hat{Q}(q^+) = \frac{16\sqrt{2\pi}\alpha_s}{N_c} \int \frac{d^4y d^4k}{(2\pi)^4} e^{iky} q^+ (M|\text{Tr}[F^{1\mu}(0) F^{+\mu}(y)]|M) \frac{(q+k)^2}{(q+k)^2 + i\epsilon},$$

(6.8)

where $|M\rangle$ represents the medium state given by Eq. 6.3. We do an analytic continuation of $\hat{Q}$ in a $q^+$ complex-plane. We note that the above quantity $\hat{Q}$ has a branch cut due to the quark propagator having momentum $q + k$ in a region where $q^+ \sim T \ll q^-$. In this region, the incoming hard parton is on-shell $q^2 = 2q^+ q^- \approx 0$. Moreover, we can show that

$$\frac{\text{Disc}[\hat{Q}(q^+)]}{2\pi i} \bigg|_{at \ q^+ \sim T} = \hat{q}.$$  

(6.9)

We also note that there is an additional discontinuity in the region $q^+ \in (0, \infty)$ due to vacuum-like radiative processes. In this region, the hard parton is time-like and $q^2 = 2q^+ q^- > 0$. However, when one takes $q^+ \ll 0$, say $q^+ = -q^-$, the discontinuity $\text{Disc}[\hat{Q}(q^+)]|_{q^+ \sim -q^-}$ vanishes and one can expand the quark propagator as follows:

$$\frac{1}{(q + k)^2} \sim \frac{1}{2q^- (-q^- + (k^+ - k^-))} = -\frac{1}{2(q^-)^2} \left[ \sum_{n=0}^{\infty} \left( \frac{\sqrt{2}k_z}{q^-} \right)^n \right].$$

(6.10)
In above expression, we can replace the gluon momentum $k_z$ with regular derivative $\partial_z$ acting on the Field-Strength $F_{\perp \mu}^+(y)$. To include the contributions from gluon scattering diagrams, we promote the regular derivative $\partial_z$ into a covariant derivative $D_z$. Thus, we arrive at

$$\hat{Q}(q^+ = -q^-) = \frac{8\sqrt{2}\pi\alpha_s}{N_c q^-} \langle M | \text{Tr}[F^+_{\perp \mu}(0)] \sum_{n=0}^{\infty} \left( \frac{i\sqrt{2}D_z}{q^-} \right)^n F^+_{\perp \mu}(0) | M \rangle. \quad (6.11)$$

In the above equation, each term in the series is local, and hence, one can directly compute their expectation value on the thermal lattices. Note that $\hat{Q}(q^+ = -q^-)$ is not the transport coefficient $\hat{q}$, however, both are related.

Next, to relate $\hat{Q}$ to physical $\hat{q}$, we consider the following contour integral in the $q^+$ complex-plane:

$$I_1 = \oint_{C_1} dq^+ \frac{\hat{Q}(q^+)}{2\pi i (q^+ + q^-)}, \quad (6.12)$$

where the contour $C_1$ shown in Fig. 6.2 is a dotted circle (counter-clockwise direction) centered around point $q^+ = -q^-$ and with a radius small enough to exclude regions where $\hat{Q}(q^+)$ may have discontinuity. Using Cauchy-Goursat theorem, one can evaluate the integral as $I_1 = \hat{Q}(q^+ = -q^-)$. Now, we deform the contour $C_1$ into $C_2$ and extend it to infinity. The integral over semi-circles in upper and lower plane goes to zero. Thus, the contribution to the integral mainly comes from the integral over the branch cut $q^+ \in (-T_1, \infty)$:

$$\hat{Q}(q^+ = -q^-) = \int_{-T_1}^{T_2} dq^+ D\text{isc}[\hat{Q}(q^+)] + \int_{T_2}^{\infty} dq^+ D\text{isc}[\hat{Q}(q^+)] + \int_{0}^{\infty} dq^+ D\text{isc}[\hat{Q}(q^+)] + \int_{-T_1}^{\infty} dq^+ D\text{isc}[\hat{Q}(q^+)], \quad (6.13)$$

where the first integral represents the contributions purely from thermal discontinuity and second integral represents the contribution purely from vacuum discontinuity in $\hat{Q}(q^+)$ on $q^+$ real-axis.

The limits $-T_1$ and $T_2$ in the first integral (Eq. 6.13) represents lower bound and upper bound of $q^+$, beyond which the thermal discontinuity in $\hat{Q}(q^+)$ on $q^+$ real-axis is zero. In this region, the hard parton is close to on-shell, i.e. $q^2 = 2q^+q^- \approx 0$ and undergoes scattering
with the medium. The discontinuity in this region is related to physical $\hat{q}$ via relation given in Eq. 6.9. The second integral in Eq. 6.13 represents the contribution from a vacuum-like processes, where the hard quark with momentum $q^+ \in (0, \infty)$ is time-like and can undergo vacuum-like splitting. Thus, this second integral is temperature independent.

At this point, we employ Eq. 6.9 to arrive at following expression of the average $\hat{q}$ given as

$$\hat{q} = \frac{8\sqrt{2}\pi\alpha_s}{N_c(T_1 + T_2)} \langle M | [F^{+\perp\mu}(0) \sum_{n=0}^{\infty} \left( \frac{i\sqrt{2}D_z}{q^-} \right)^n F^{+\perp\mu}_n(0)] | M \rangle_{\text{(Thermal–Vacuum)}} \rangle. \quad (6.14)$$

The above expression is a desired form of transport coefficient $\hat{q}$ suitable for lattice calculation which contains several features. First, each of the terms in the series are local, that means one can hope to compute their expectation value on the thermal lattice. Second, higher order terms in the series are suppressed by the hard scale $q^-$, and hence, computing the first few terms may be sufficient. Also, we emphasize that we have not made any assumptions regarding the constituents of the plasma, and hence, the expression of the transport
coefficient \( \hat{q} \) given in Eq. [6.14] is valid for both pure gluonic thermalized plasma and full quark-gluon thermalized plasma. The term \( T_1 + T_2 \sim T \) (Eq. [6.14]) represents the width of the thermal discontinuity in \( \hat{Q}(q^+) \) on \( q^+ \) real-axis. It is also interesting to mention that a similar kind of operator product expansion has been found by the author of Ref. [133] in the analysis of the parton distribution function on an Euclidean space.

6.2 Expression of Field-Strength Field-Strength correlators in \( \hat{q} \) series

In this study, we have attempted to compute operators upto order \( n = 4 \) in \( \hat{q} \) series (Eq. [6.14]) and ignored higher-order terms. At \( n = 0 \) and \( n = 1 \), the correlators are \( \langle M | \text{Tr}[F^{+\perp}_\mu(0) F^{+\perp}_{\perp\mu}(0)] | M \rangle \) and \( \langle M | \text{Tr}[F^{+\perp}_\mu(0) \left( \frac{i\sqrt{2}D_i}{q^+} \right) F^{+\perp}_{\perp\mu}(0)] | M \rangle \). But, we note that these operators and higher-order operators are in Minkowski space. In order to compute their expectation value on the lattice, we rotate the operator products to Euclidean space. This is achieved by following transformations:

\[
x^0 \rightarrow -ix^4, \quad A^0 \rightarrow iA^4 \quad \Rightarrow \quad F^{0i} \rightarrow iF^{4i}. \quad (6.15)
\]

The first operator \((n = 0)\) in the expansion is \( \langle M | F^{+\mu}_{\perp}(0) F^{+\mu}_{\perp}(0) | M \rangle \) which can written
in following form:

\[
F^+_{\perp \mu} (0) F^+_{\perp \mu} (0) = \left[ \partial^\mu A^\perp (0) - \nabla^\mu A^+ (0) \right] \left[ \partial^\mu A^\perp (0) - \nabla^\mu A^+ (0) \right]
\]

\[
= \left[ \left( \frac{\partial^0 + \partial^3}{\sqrt{2}} \right) A^i (0) - \partial^i \left( \frac{A^0 + A^3}{\sqrt{2}} \right) \right] \left[ \left( \frac{\partial^0 + \partial^3}{\sqrt{2}} \right) A_i (0) - \partial_i \left( \frac{A^0 + A^3}{\sqrt{2}} \right) \right]
\]

where, \( i = 1, 2 \)

\[
= \frac{1}{2} \left[ \left( \partial^0 A^i - \partial^i A^0 \right) + \left( \partial^3 A^i - \partial^i A^3 \right) \right] \left[ \left( \partial^0 A_i - \partial_i A^0 \right) + \left( \partial^3 A_i - \partial_i A^3 \right) \right]
\]

\[
= \frac{1}{2} \left[ F^{0i} + F^{3i} \right] \left[ F^0_i + F^3_i \right]
\]

changing \( t \rightarrow -i \tau \) & \( A^0 \rightarrow i A^4 \Rightarrow F^{0i} \rightarrow i F^{4i} \)

\[
= \frac{1}{2} \left[ (i F^{41} + F^{31}) (i F^4 + F^3) + (i F^{42} + F^{32}) (i F^2 + F^3) \right]
\]

\[
= \sum_{i=1, 2} \frac{1}{2} \left[ F^{3i} F^{3i} - F^{4i} F^{4i} \right] + i \sum_{i=1, 2} F^{4i} F^{3i}.
\]

(6.16)

The first operator above \( \sum_{i=1, 2} [F^{3i} F^{3i} - F^{4i} F^{4i}] \) (Eq. 6.16) within the square bracket is a symmetric operator and represents \( \sum_{i=1, 2} E^2_i + B^2_i \), where \( \vec{E} \) and \( \vec{B} \) are chromo-electric field and chromo-magnetic field, respectively. The second operator above \( \sum_{i=1, 2} [F^{4i} F^{3i}] \) (Eq. 6.16) is a anti-symmetric operator and represents \( (\vec{E} \times \vec{B})_z \), the \( z \)-component of the Poynting vector for chromo-electric and magnetic fields.

The operators at \( n = 1 \) is given by

\[
\begin{align*}
F^+_{\perp \mu} \left( \frac{i \sqrt{2} D_z}{q^-} \right) F^+_{\perp \mu} & \longrightarrow \frac{\sqrt{2} i}{2q^-} \left[ \sum_{i=1}^2 \left( F^{3i} D_z F^{3i} - F^{4i} D_z F^{4i} \right) + i \sum_{i=1}^2 \left( F^{4i} D_z F^{3i} + F^{3i} D_z F^{4i} \right) \right],
\end{align*}
\]

(6.17)

where \( D_z \) is the first-order covariant derivative along the \( z \)-direction. The operators at \( n = 2 \)
is given by

\[ F^{+\mu} \left( \frac{i\sqrt{2}D_z}{q^-} \right)^2 F^{\perp \mu} \rightarrow \frac{-1}{(q^-)^2} \left[ \sum_{i=1}^{2} (F^{3i} D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}) + i \sum_{i=1}^{2} (F^{4i} D_z^2 F^{3i} + F^{3i} D_z^2 F^{4i}) \right], \]

(6.18)

where \( D_z^2 \) is the second-order covariant derivative along the \( z \)-direction. The operators at \( n = 3 \) is given by

\[ F^{+\mu} \left( \frac{i\sqrt{2}D_z}{q^-} \right)^3 F^{\perp \mu} \rightarrow \frac{-i\sqrt{2}}{(q^-)^3} \left[ \sum_{i=1}^{2} (F^{3i} D_z^3 F^{3i} - F^{4i} D_z^3 F^{4i}) + i \sum_{i=1}^{2} (F^{4i} D_z^3 F^{3i} + F^{3i} D_z^3 F^{4i}) \right], \]

(6.19)

where \( D_z^3 \) is the third-order covariant derivative along the \( z \)-direction. The operators at \( n = 4 \) is given by

\[ F^{+\mu} \left( \frac{i\sqrt{2}D_z}{q^-} \right)^4 F^{\perp \mu} \rightarrow \frac{2}{(q^-)^4} \left[ \sum_{i=1}^{2} (F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}) + i \sum_{i=1}^{2} (F^{4i} D_z^4 F^{3i} + F^{3i} D_z^4 F^{4i}) \right], \]

(6.20)

where \( D_z^4 \) is the fourth-order covariant derivative along the \( z \)-direction.

In this thesis, operators listed above will be calculated. For terms upto \( n = 4 \) in the \( \hat{q} \) series, it will be argued that there are only three operators that have non-zero value; these are \( \sum_{i=1}^{2} (F^{3i} F^{3i} - F^{4i} F^{4i}) \), \( \sum_{i=1}^{2} (F^{3i} D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}) \) and \( \sum_{i=1}^{2} (F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}) \).

The covariant derivatives are defined as

\[ D_z^2 F_{\mu\nu} = \frac{1}{a^2} \left[ U_z(z; z + a) F_{\mu\nu}(z + a) U_z^\dagger(z; z + a) + U_z^\dagger(z; z - a) F_{\mu\nu}(z - a) U_z(z - a; z) - 2 F_{\mu\nu}(z) \right] \]

(6.21)
and

\[
D_z^4 F_{\mu\nu} = \frac{1}{a^4} \left[ U_z(z; z + a) U_z(z + a; z + 2a) F_{\mu\nu}(z + 2a) U_z^\dagger(z + a; z + 2a) U_z^\dagger(z; z + a) \\
+ U_z^\dagger(z - a; z) U_z^\dagger(z - 2a; z - a) F_{\mu\nu}(z - 2a) U_z(z - 2a; z - a) U_z(z - a; z) \\
- 4 U_z(z; z + a) F_{\mu\nu}(z + a) U_z^\dagger(z; z + a) \\
- 4 U_z^\dagger(z - a; z) F_{\mu\nu}(z - a) U_z(z - a; z) \\
+ 6 F_{\mu\nu}(z) \right].
\]

(6.22)

In lattice perturbation theory, to improve the convergence of the operators, one follows tadpole improvement prescription in which the lattice artifacts that arise from the tadpole diagrams are largely cancelled by the tadpole improvement [134–136]. In this prescription, the link \( U_\mu \)'s are divided by the mean link \( u_0 \), i.e.

\[
U_\mu(x) \to \frac{U_\mu(x)}{u_0},
\]

(6.23)

where the mean link \( u_0 = < AP >^{1/4} \) is defined as fourth-root of average plaquette. To incorporate this feature, we define tadpole improved version of the covariant derivatives:

\[
D_z^2 F_{\mu\nu} = \frac{1}{a^2} \left[ \frac{1}{u_0^2} \left\{ U_z(z; z + a) F_{\mu\nu}(z + a) U_z^\dagger(z; z + a) + U_z^\dagger(z - a; z) F_{\mu\nu}(z - a) U_z(z - a; z) \right\} \\
- 2 F_{\mu\nu}(z) \right].
\]

(6.24)
and

\[
D_z^4 F_{\mu\nu} = \frac{1}{a^4} \left[ \frac{1}{u_0^4} \left\{ U_z(z; z + a) U_z(z + a; z + 2a) F_{\mu\nu}(z + 2a) U_z^\dagger(z + a; z + 2a) U_z^\dagger(z; z + a) \right. \\
+ U_z(z - a; z) U_z^\dagger(z - 2a; z - a) F_{\mu\nu}(z - 2a) U_z(z - 2a; z - a) U_z(z - a; z) \bigg\} \\
- \frac{4}{u_0^4} \left\{ U_z(z; z + a) F_{\mu\nu}(z + a) U_z^\dagger(z; z + a) \right. \\
+ U_z(z - a; z) F_{\mu\nu}(z - a) U_z(z - a; z) \bigg\} \\
+ 6 F_{\mu\nu}(z) \right].
\]

(6.25)

To compute the local operators, we set up a four-dimensional (4D) grid, specified by the coordinate \( x_\mu = a_L \ast n_\mu \), where \( n_\mu = (n_x, n_y, n_z, n_\tau) \) is a 4-component Euclidean vector. Here \( n_x, n_y, n_z, n_\tau \) represents the number of grid points in \( x, y, z, \) and \( \tau \) direction. We denote \( a_L \) to represent the lattice spacing. Then, the temperature is given by \( T = 1/n_\tau a_L \).

In our calculations, lattices with the same lattice spacing in all directions are employed. We consider the lattice to be symmetric in the spatial directions, i.e. \( n_x = n_y = n_z = n_s \). For calculations at finite temperature, the number of sites in the spatial direction \( (n_s) \) is set to be four times the number of sites in the temporal direction \( (n_\tau) \), whereas vacuum calculations are done with the same number of sites in all four directions.

### 6.3 Comparison of clover-definition vs single-plaquette definition for \( F_{\mu\nu} \)

In order to evaluate the Euclidean operators in Eq. (6.14) one need to express the field-strength operator in terms of the link variables. A general discretization of the field-strength tensor in terms of the link variables is given by the [see figure 6.3(a)],

\[
F_{\mu\nu}(x) = \frac{1}{2i g a^2} \left[ U_{\mu,\nu}(x) - U_{\mu,\nu}^\dagger(x) - \frac{1}{3} \text{Tr}(U_{\mu,\nu}(x) - U_{\mu,\nu}^\dagger(x)) \right],
\]

(6.26)

where \( g \) is the bare lattice coupling constant, \( a \) is the lattice spacing and \( U_{\mu,\nu} \) is a plaquette operator (1 \times 1 square-loop) representing the product of the four links in \( \mu - \nu \) plane.
We shall refer to this definition as single-plaquette method of computing $F_{\mu\nu}(x)$. In the above equation, in order to enforce the traceless property of the Gell-Mann matrices (SU(3) generators), we have subtracted the one-third of the trace.

Using algebraic manipulations, one can express plaquette operator $U_{\mu\nu}$ as

$$U_{\mu,\nu}(x) = \exp[iga^2 F_{\mu\nu}(x) + \frac{iga^3}{2} \{\partial_{\mu} + \partial_{\nu}\} F_{\mu\nu}(x) + O(ga^4) + O(g^2)].$$  \hspace{1cm} (6.27)$$

Thus,

$$U_{\mu,\nu}(x) - U_{\mu,\nu}^\dagger(x) = 2iga^2 F_{\mu\nu}(x) + iga^3 \{\partial_{\mu} + \partial_{\nu}\} F_{\mu\nu}(x) + O(ga^4).$$ \hspace{1cm} (6.28)$$

This indicate that the single-plaquette definition of $F_{\mu\nu}$ contains the contribution from the $O(ga^3)$ and $O(ga^4)$ terms.

A more popular discretization of the field strength tensor in terms of the link variables is given by the clover-leaf diagram (see Fig. 6.3(b)). In this clove-leaf approach, $F_{\mu\nu}$ is given as

$$F_{\mu\nu}(x) = \frac{1}{2iga^2} \frac{1}{4} \left[ Q_{\mu\nu}(x) - Q_{\mu\nu}^\dagger(x) - \frac{1}{3} \text{Tr}(Q_{\mu\nu}(x) - Q_{\mu\nu}^\dagger)(x) \right],$$ \hspace{1cm} (6.29)$$

where $Q_{\mu\nu}(x) = U_{\mu,\nu}(x) + U_{-\mu,\nu}(x) + U_{-\mu,-\nu}(x) + U_{\mu,-\nu}(x)$ represents the sum over four plaquettes around the site $x$ in the $\mu$-$\nu$ plane. In the above equation, in order to enforce the traceless property of the Gell-Mann matrices (SU(3) generators), we have subtracted one-third of the trace.

The plaquette operator $U_{\mu,\nu}(x)$ for the top-left $1 \times 1$ square [Fig. 6.3(b)] can be written as

$$U_{-\mu,\nu}(x) = \exp[iga^2 F_{\mu\nu}(x) + \frac{iga^3}{2} \{-\partial_{\mu} + \partial_{\nu}\} F_{\mu\nu}(x) + O(ga^4) + O(g^2)].$$ \hspace{1cm} (6.30)$$

The plaquette operator $U_{\mu,\nu}(x)$ for the bottom-left $1 \times 1$ square [Fig. 6.3(b)] can be written
as

\[ U_{\mu,\nu}(x) = \exp[iga^2 F_{\mu\nu}(x) + \frac{iga^3}{2} \{-\partial_\mu - \partial_\nu\} F_{\mu\nu}(x) + O(ga^4) + O(g^2)]. \quad (6.31) \]

The plaquette operator \( U_{\mu\nu} \) for the bottom-right \( 1 \times 1 \) square [Fig. 6.3(b)] can be written as

\[ U_{\mu,\nu}(x) = \exp[iga^2 F_{\mu\nu}(x) + \frac{iga^3}{2} \{-\partial_\mu - \partial_\nu\} F_{\mu\nu}(x) + O(ga^4) + O(g^2)]. \quad (6.32) \]

Now, adding the contributions from four-leaves of the clover, we get

\[ Q_{\mu\nu}(x) - Q_{\mu\nu}^\dagger(x) = 2iga^2 F_{\mu\nu}(x) + O(ga^4). \quad (6.33) \]

The above expression shows that the clover-definition of \( F_{\mu\nu} \) removes the \( O(ga^3) \) discretization error and leads to an improved accuracy of \( O(ga^4) \).

Figure 6.3: (a) Single-plaquette definition of \( F_{\mu\nu} \). (b) Clover-definition of \( F_{\mu\nu} \).

To compare the two definitions, we show expectation value (vacuum subtracted) of

\[ \sum_{i=1}^{2} (F^{3i} F^{3i} - F^{4i} F^{4i}) \quad \text{and} \quad \sum_{i=1}^{2} (F^{3i} F^{4i} + F^{4i} F^{3i}) \]

operators scaled by \( T^4 \) in Fig. 6.4 for the case of pure SU(3) gauge. The underlying details of the calculation including the input lattice settings will be discussed in the later sections. From the plot, we see that for the sym-
Figure 6.4: Comparison of FF operators for two different definition of $F_{\mu\nu}$: one using single-plaquetter and the other using clover-leaf method. (a) Vacuum subtracted expectation value of operator $\text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] / T^4$. (b) Vacuum subtracted expectation value of operator $\text{Tr}[F^{3i}F^{4i} + F^{4i}F^{3i}] / T^4$.

metric operator, the temperature dependence is qualitatively similar between clover-method and single-plaquette method. In Fig. 6.4(b), the expectation value of the anti-symmetric operator is zero for clover-method but has non-zero rising behaviour at lower temperatures for single-plaquette method. This difference in the qualitative behaviour of the anti-symmetric operator arising from the different prescriptions of $F_{\mu\nu}$ is mainly due the discretization error in the expressions of $F_{\mu\nu}$ (Eq. 6.33, 6.28,6.29,6.26).

In general, under parity ($P$) and time-reversal ($T$), the operators transform as

$$
F^{3i} \rightarrow F^{3i}; \quad F^{4i} \rightarrow -F^{4i}; \quad D_z \rightarrow D_z;
$$

$$
F^{3i} \rightarrow -F^{3i}; \quad F^{4i} \rightarrow F^{4i}; \quad D_z \rightarrow D_z;
$$

(6.34)

Based on the above properties, we can say that the symmetric term $\sum_{i=1}^{2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i})$ is even under both parity and time-reversal transformations, however, the anti-symmetric operator $\sum_{i=1}^{2} \text{Tr}(F^{3i}F^{4i} + F^{4i}F^{3i})$ is odd under parity as well as time-reversal. Therefore, the gauge invariant average of the anti-symmetric operator $\sum_{i=1}^{2} \text{Tr}(F^{3i}F^{4i} + F^{4i}F^{3i})$ should
be zero. Indeed, we observe this in the plot 6.4(b). The single-plaquette definition of \( F_{\mu\nu} \) suffer from discretization error \( O(ga^3) \) which is an odd power in the lattice spacing, whereas the clover-definition does not contain \( O(ga^3) \) and leads to an overall improved accuracy of \( O(ga^4) \). Also, it is important to note that the \( O(ga^3) \) term leads to the imaginary part of \( \hat{q} \) and hence, represents an unphysical term. This leads us to the conclusion that the clover-definition is a better choice compared to the single-plaquette definition to compute \( F_{\mu\nu} \) in terms of the link variables.

Moreover, we would like to point out that most of the operators listed in Eq. 6.16, 6.17, 6.18, 6.19 and 6.20 are not even under parity and time-reversal. In fact, only the operators \( \sum_{i=1}^{2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i}) \), \( \sum_{i=1}^{2} \text{Tr}(F^{3i}D_z^2F^{3i} - F^{4i}D_z^2F^{4i}) \) and \( \sum_{i=1}^{2} \text{Tr}(F^{3i}D_z^4F^{3i} - F^{4i}D_z^4F^{4i}) \) are even under parity and time-reversal, and rest of them are odd either under parity or time-reversal transformations. Thus, in the remaining portion of this chapter, we shall only consider the clover-definition of \( F_{\mu\nu} \) and evaluate following three non-zero operators: \( \sum_{i=1}^{2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i}) \), \( \sum_{i=1}^{2} \text{Tr}(F^{3i}D_z^2F^{3i} - F^{4i}D_z^2F^{4i}) \) and \( \sum_{i=1}^{2} \text{Tr}(F^{3i}D_z^4F^{3i} - F^{4i}D_z^4F^{4i}) \).

### 6.4 Evaluating operators for SU(2) quenched plasma

For SU(2) quenched plasma, the field-strength field-strength (FF) correlators were first estimated by A. Majumder in Ref. [12]. The figure 6.5 shows the lattice calculation of \( \sum_{i=1}^{2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i}) \) operator as a function of lattice bare coupling \( g \) (left) and also as a function of temperature \( T \) (right). This calculation was performed by taking statistical average over 5000 gauge configurations which were generated using the SU(2) heat-bath algorithm (Chapter 5 section 5.2.1). The scale was set on the lattice using the two-loop perturbative renormalization group (RG) equation with non-perturbative correction factor \( \lambda(g^2) \) given as:

\[
a_L = \frac{\lambda(g^2)}{\Lambda_L} \left( \frac{11g^2}{24\pi^2} \right)^{-\frac{g_1}{2g_4}} \exp \left( -\frac{12\pi^2}{11g^2} \right),
\]

where \( g \) represents the bare lattice coupling and \( \Lambda_L \) is a parameter set to \( \Lambda_L = 10.3 \) MeV. The free parameter \( \lambda(g^2) \) is adjusted such that \( T_c/\Lambda_L \) is independent of the bare coupling.
constant $g$. The temperature of the lattice is obtained by $T = 1/(n_\tau a)$. Fig. 6.5(a) shows the “thermal+vacuum” and “vacuum” expectation value of the symmetric correlator $\sum_{i=1,2} a^4 \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i})/2$ as a function of the lattice bare coupling $\beta_0 = 4/g^2$. We see that the vacuum expectation value is close to zero for all values of the bare coupling $\beta_0$.

Fig. 6.5(b) shows the temperature dependence of the expectation value of the symmetric correlator $\sum_{i=1,2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i})/(2T^4)$. We note that the phase transition is around $T_c \sim 250-350$ MeV. We also note that the symmetric correlator starts to scale as $T^4$ for temperatures above $1.25-2T_c$.

![Figure 6.5](image)

**Figure 6.5:** Pure SU(2) quenched lattice calculation. (a) Expectation value of $\sum_{i=1,2} a^4 \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i})/2$ as a function of $\beta_0 = 4/g^2$. (b) Expectation value of $\sum_{i=1,2} \text{Tr}(F^{3i}F^{3i} - F^{4i}F^{4i})/2$ correlator scaled by $T^4$.

### 6.5 Evaluating operators for SU(3) quenched plasma

In this section, we compute local Field-Strength-Field-Strength (FF) operators, for a more realistic case of SU(3) quenched plasma. We generated SU(3) gauge field configurations using the public version of Multiple Instruction & multiple data (MIMD) Lattice Computation (MILC) code package \cite{43,44}. The gauge action used is standard Wilson’s gauge action. The thermal configurations are generated for lattice sizes $n_\tau = 4, 6$ and 8.
with the aspect ratio $n_s/n_\tau = 4$, whereas the corresponding vacuum configurations are generated with $n_\tau = n_s$. All the calculations have been done by taking a statistical average over 10000 gauge configurations generated using the standard heat-bath algorithm, as outlined in section 5.2.2. The MILC code was built against Scientific Discovery through Advanced Computing (SciDAC) packages, namely QMP (message passing), QIO (file I/O), QLA (linear algebra), QDP/c (data parallel), QOPQDP/c (optimized higher-level code) [137]. These optimization routines significantly accelerated the performance of the code. We performed lattice calculation over a wide range of temperatures, $200 < T < 860 \text{ MeV}$.

For $n_\tau = 4$, the temperature $T = 200 \text{ MeV}$ corresponds to the lattice spacing $a = 0.25 \text{ fm}$, whereas $T = 800 \text{ MeV}$ corresponds to the lattice spacing $a = 0.06 \text{ fm}$. For $n_\tau = 6$, the temperature $T = 200 \text{ MeV}$ corresponds to the lattice spacing $a = 0.17 \text{ fm}$, whereas $T = 800 \text{ MeV}$ corresponds to the lattice spacing $a = 0.04 \text{ fm}$. For $n_\tau = 8$, the temperature $T = 200 \text{ MeV}$ corresponds to the lattice spacing $a = 0.125 \text{ fm}$, whereas the $T = 800 \text{ MeV}$ corresponds to the lattice spacing $a = 0.03 \text{ fm}$. The spatial length ($L$) of the box is set by the temperature $T$ and in our case given as $L = 4/T$. The temperature $T = 200 \text{ MeV}$ corresponds to a box with spatial length 4 fm, whereas $T = 800 \text{ MeV}$ corresponds to a box with spatial length 1 fm. The input parameter $\beta_0$ is given as

$$
\beta_0 = 2N_c/g_0^2 = 6/g_0^2, \quad (6.36)
$$

where $g_0$ is the lattice bare coupling constant. As pointed out in section 6.3, the FF operators were calculated using the clover-leaf definition of $F_{\mu\nu}$ as given in Eq. 6.29.

### 6.5.1 Bare operators

We have computed FF correlators for lattice sizes $n_\tau = 4, 6$ and 8 as function of input parameter $\beta_0 = 6/g_0^2$ (Fig. 6.6, 6.7 and 6.8). In Fig. 6.6(a), we show the expectation value of the operator $g_0^2a^4 \sum_{i=1,2} \langle \text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] \rangle$ as a function of $\beta_0$ for $n_\tau = 4$. The thermal+vacuum expectation (in red color) value shows a rapid transition in the region $\beta_0 \in (5.5, 6.0)$ and has
negligible contributions from vacuum processes (in blue color). The plot in the center [Fig. 6.6(b)] represents the expectation value of the operator $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr} [F^3_i D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle$. We computed the thermal + vacuum (black color) and pure vacuum (green color) expectation value in absence of the tadpole corrections for the link $U_\mu$ in the covariant derivative $D_z$ (Eq. 6.21). We also computed the thermal + vacuum (red color) and pure vacuum (blue color) expectation value in the presence of the tadpole correction factors (Eq. 6.24).

We observe that the thermal+vaccum and pure vaccum results are approximately same in the magnitude indicating that the pure thermal contributions are much smaller than the pure vacuum results. We also note that for a given bare coupling $\beta$, both the thermal+vacuum and pure vacuum expectation value enhances by the same factor as one adds tadpole correction factors in the calculation of the covariant derivative. In Fig. 6.6(c), we show the expectation value of the operator $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr} [F^3_i D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle$ as a function of $\beta_0$. Here as well, the vacuum contributions are most dominant. We also computed the expectation value of $g_0^8 a^4 \sum_{i=1,2} \langle \text{Tr} [F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle$, $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr} [F^3_i D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle$ and $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr} [F^3_i D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle$ for $n_\tau = 6$ (Fig. 6.7) and $n_\tau = 8$ (Fig. 6.8), and have observed trend similar to the case of $n_\tau = 4$.

### 6.5.2 Scale setting for SU(3) quenched lattices

To understand the behavior of these operators in terms of physical quantities, we need to relate the bare coupling constant with the lattice spacing. This relation is set using the two-loop perturbative renormalization group (RG) equation with non-perturbative correction given as

$$a = \frac{f(\beta_0)}{\Lambda_L} \left[ \frac{11g_0^2}{16\pi^2} \right]^{\frac{331}{128}} \exp \left[ -\frac{8\pi^2}{11g_0^2} \right]$$

(6.37)

where $\Lambda_L$ is a dimensionful lattice parameter, $\beta_0 = 6/g_0^2$, and $f(\beta_0)$ is non-perturbative correction. We define

$$W(\beta_0) = \left[ \frac{11g_0^2}{16\pi^2} \right]^{\frac{331}{128}} \exp \left[ -\frac{8\pi^2}{11g_0^2} \right]$$

(6.38)

Note, the temperature $T$ is obtained by $1/(n_\tau a)$. We parametrize non-perturbative correction...
Figure 6.6: FF correlators in pure $SU(3)$ plasma for lattice size $n_T=4$, $n_s=16$. (a) Thermal + Vacuum (red color) and pure vacuum (blue color) expectation value of $g_s^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle$. (b) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_s^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_{\mu}$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in presence of tadpole factors. (c) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_s^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_{\mu}$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in the presence of the tadpole factors.

For a given lattice of size $n_T \times n_s^3$, we compute the expectation value of the Polyakov loop and obtained the critical coupling $\beta_c = 6/g_s^2$. Thus, the critical temperature $T_c$ can be related to $\beta_c$ via $T_c = 1/(n_T a_c)$, where $a_c = a(\beta_c)$. We evaluate the function $f(\beta_0)$ at the critical coupling using

$$f(\beta_c) = \frac{1}{n_T W(\beta_c) T_c} \Lambda_L$$

(6.40)

To determine the critical coupling $\beta_0$ for different $n_T$s, we study the behavior of the Polyakov loop as a function of $\beta_0$. The expectation value of the Polyakov loop ($P$) for a given gauge
Figure 6.7: FF correlators in pure $SU(3)$ plasma for lattice size $n_\tau=6$, $n_s=24$. (a) Thermal + Vacuum (red color) and pure vacuum (blue color) expectation value of $g_0^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F^3_{3i} F^{3i} - F^4_{i} D^2_{4i} F^{4i}] \rangle$. (b) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F^3_{3i} D^2_{z} F^{3i} - F^4_{4i} D^2_{2i} F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_{\mu}$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in presence of tadpole factors. (c) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F^3_{3i} D^4_{z} F^{3i} - F^4_{4i} D^4_{2i} F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_{\mu}$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in the presence of the tadpole factors.

configuration is given as

$$P = \frac{1}{n_x n_y n_z} \text{tr} \left[ \sum_{n=0}^{n_\tau-1} \prod_{\vec{r}} U_4(na, \vec{r}) \right],$$  \hspace{1cm} (6.41)$$

where $U_4(na, \vec{r})$ is a gauge link in the temporal $(\tau)$ direction.

In Fig. 6.9(a), we show the vacuum subtracted expectation value of the Polyakov loop $\langle |P| \rangle$ as a function of bare coupling $\beta_0$. From the Polyakov loop calculation, the critical coupling for lattice sizes $n_\tau = 4, 6$ and 8 comes out to be 5.69, 5.89 and 6.06, respectively. The critical coupling for higher lattice sizes $n_\tau=10, 12, 14, 16, 18, 20, 22$ were taken from Refs [139] which are 6.2, 6.33, 6.44, 6.54, 6.63, 6.71 and 6.79, respectively. We estimated the non-perturbative correction factor $f(\beta_0)$, by fitting the data obtained using Eq. 6.40 and adjusting the free parameters in $f(\beta_0)$ (Eq. 6.39) such that $T_c/\Lambda_L$ is independent of bare coupling constant $g$. Each blue points in Fig. 6.9(b) represents $f(\beta_c)$ for a corresponding
value of $\beta_c$, where as the red line is the fit to the data points. In this extraction, we set the critical temperature to $T_c \approx 265$ MeV ($\text{pure } SU(3) \text{ gauge } [140]$) and lambda parameter $\Lambda_L = 5.5$ MeV ($[141-143]$).

The extracted value of fit parameters are

$$c_0 = -23.2088; \quad c_1 = 0.993504; \quad c_2 = -25.2466; \quad c_3 = 0.90595. \quad (6.42)$$

Using above parameters, we plot lattice spacing $a$ (Eq. 6.37) as a function of $\beta_0$ [see Fig. 6.9(c)]. We also show the vacuum subtracted expectation value of the Polyakov loop as a function of temperature for $n_s = 4, 6$ and 8. The green vertical line represents the critical temperature for pure $SU(3)$ gauge theory.
Figure 6.9: Scale setting for pure SU(3) gauge case. (a) The vacuum subtracted expectation value of the Polyakov loop at \( n_\tau = 4, 6 \) and 8 with \( n_s = 4n_\tau \). (b) Plot of \( f(\beta_c) \) as a function of critical coupling \( \beta_c \). The red line shows the fit to the data points where a parametrization given in Eq. 6.39 is used as the fit function. (c) The plot of lattice spacing \( a(\text{MeV}^{-1}) \) as a function of the bare coupling \( \beta_0 = 6/g_0^2 \) using parameters extracted from fits to \( f(\beta_c) \) [see Fig. 6.9(b)]. (d) The vacuum subtracted expectation of the Polyakov loop \( \langle |P| \rangle \) as a function of \( T \). The green vertical line represents the critical temperature \( T_c \approx 265 \) for pure SU(3) gauge theory.

6.5.3 Temperature dependence of vacuum subtracted operators

We present the vacuum subtracted expectation value of FF correlators as a function of temperature in Fig. 6.10(a), 6.10(b) and 6.10(c) for \( n_\tau = 4, 6 \) and 8, respectively. In all three
plots, the red points represent the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle$ scaled by $T^4$ to make it dimensionless. The points in blue color represents the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle$ scaled by $T^4(q^-)^2$ to make it dimensionless. The factor $(q^-)^2$ is used because a quadratic power of the hard scale $q^-$ appears in the denominator of the second-order FF correlator term. This allows us to estimate relative strength between the operators at $n = 0$ and $n = 2$ in the $\hat{q}$ series (Eq. 6.14). The points in black color represents the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}] \rangle$ scaled by $T^4(q^-)^4$. As quartic power of $q^-$ appears in the FF correlators at $n = 4$ in the $\hat{q}$ series, the operator is scaled by 4th-power of $q^-$. The hard quark light-cone energy $q^-$ is set 100 GeV. These calculations include the tadpole improvement for the link $U_\mu$ in the covariant derivative.

Our calculations show that the operator $\sum_{i=1,2} \langle \text{Tr}[F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle / T^4$ (red color) is dominant among all three operators. The FF correlator term with the second-order covariant derivative is suppressed by a factor of $10^3$, whereas the term with the fourth-order covariant derivative is suppressed by a factor of $10^6$ relative to the operator in red color. Overall, we observe that the zeroth-order term $\langle \text{Tr}[F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle$ (red curve) exhibit a rapid transition near the critical temperature $T \in (250, 350)$ MeV and is dominant at high temperature relative to rest of the operators.

6.6 Evaluating operators for 2+1 flavor SU(3) plasma

In this section, we compute local Field-Strength-Field-Strength (FF) operators for the case of quark-gluon plasma. The gauge field configurations are generated using public version of Multiple Instruction & multiple data (MIMD) Lattice Computation (MILC) code package \[43, 44\]. The calculation has been carried out using (2+1)-flavors of quarks, using the highly improved staggered quark action (HISQ) and tree-level Symanzik improved gauge action. This choice of action leads to discretization error $O(a^4)$ and $O(g_0^2 a^2)$. The thermal configurations generated are for lattice sizes $n_\tau = 4, 6$ and $8$ with the aspect ratio $n_s/n_\tau = 4$, whereas the corresponding vacuum configurations are generated with $n_\tau = n_s$. 
Figure 6.10: Temperature dependence of the vacuum subtracted operators $\sum_{i=1,2} \langle \text{Tr}[F^{3i} F^{4i}] \rangle / T^4$ (red color), $\sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^2 F^{3i} - F^{4i} D_z^2 F^{4i}] \rangle / (T^4(q^-)^2)$ (blue color) and $\sum_{i=1,2} \langle \text{Tr}[F^{3i} D_z^4 F^{3i} - F^{4i} D_z^4 F^{4i}] \rangle / (T^4(q^-)^4)$ (black color) in pure gluon plasma. We used $q^-$ as 100 GeV. The links in the covariant derivative are tadpole improved. (a) The real part of FF correlators for $n_\tau = 4$ and $n_s = 16$. (b) The real part of FF correlators for $n_\tau = 6$ and $n_s = 24$. (c) The real part of FF correlators for $n_\tau = 8$ and $n_s = 32$.

All the calculations have been done by taking a statistical average over 10000 gauge configurations generated using the Rational Hybrid Monte-Carlo (RHMC) algorithm. In generating the gauge configuration for (2+1)-flavor, there are three input parameters: the bare gauge coupling $\beta_0 = 10/g_0^2$, light quark masses $m_l$ (up and down), and heavier strange quark mass $m_s$.

We did not perform the tuning of the input parameters by ourselves but employed tuned input parameters (bare coupling, quark masses) published in Ref. [13, 14] by the HotQCD Collaboration and TUMQCD Collaboration. The strange quark mass $m_s$ was set to the physical value with the degenerate light quark masses $m_l = m_{u,d} = m_s/20$; in the continuum limit, this corresponds to a pion mass of about 160 MeV. The MILC code was built against Scientific Discovery through Advanced Computing (SciDAC) packages, namely QMP (message passing), QIO (file I/O), QLA (linear algebra), QDP/c (data parallel), QOPQDP/c (optimized higher-level code) [137]. These optimization routines significantly accelerated the performance of the code. We performed lattice calculation over a wide range of temperature, $150 < T < 860$ MeV. For $n_\tau = 4$, the temperature $T = 200$ MeV corresponds to the lattice...
spacing \( a = 0.25 \text{ fm} \), whereas \( T = 800 \text{ MeV} \) corresponds to the lattice spacing \( a = 0.06 \text{ fm} \). For \( n_\tau = 6 \), the temperature \( T = 200 \text{ MeV} \) corresponds to the lattice spacing \( a = 0.17 \text{ fm} \), whereas \( T = 800 \text{ MeV} \) corresponds to the lattice spacing \( a = 0.04 \text{ fm} \). For \( n_\tau = 8 \), the temperature \( T = 200 \text{ MeV} \) corresponds to the lattice spacing \( a = 0.125 \text{ fm} \), whereas the \( T = 800 \text{ MeV} \) corresponds to the lattice spacing \( a = 0.03 \text{ fm} \).

The spatial length of the box is set by the temperature \( T \) and is independent of \( n_\tau \) and \( n_s \). The temperature \( T = 200 \text{ MeV} \) corresponds to a box with spatial length 4 fm, whereas \( T = 800 \text{ MeV} \) corresponds to a box with spatial length 1 fm. The input parameter \( \beta_0 \) in the gauge action is given as

\[
\beta_0 = \frac{10}{g_0^2},
\]

(6.43)

where \( g_0 \) is the lattice bare coupling constant. As pointed out in section 6.3, the FF operators were calculated using the clover-leaf definition of \( F_{\mu\nu} \) as given in Eq. 6.29.

### 6.6.1 Bare operators

We have computed FF correlators for lattice sizes \( n_\tau = 4, 6 \) and 8 as function of input parameter \( \beta_0 = \frac{10}{g_0^2} \) (Fig. 6.11, 6.12 and 6.13). In Fig. 6.11(a), we show the expectation value of the operator \( g_0^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] \rangle \) as a function of \( \beta_0 \) for \( n_\tau = 4 \). The thermal+vacuum expectation (in red color) value shows a rapid transition in the region \( \beta_0 \in (5.5, 6.0) \) and has negligible contributions from vacuum processes (in blue color). The plot in the center [Fig. 6.11(b)] represents the expectation value of the operator \( g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F^{3i}D_z^2F^{3i} - F^{4i}D_z^2F^{4i}] \rangle \). We computed the thermal + vacuum (black color) and pure vacuum (green color) expectation value in absence of the tadpole corrections for the link \( U_\mu \) in the covariant derivative \( D_z \) (Eq. 6.21). We also computed the thermal + vacuum (red color) and pure vacuum (blue color) expectation value in the presence of the tadpole correction factors (Eq. 6.24).

We observe that the thermal+vacuum and pure vacuum results are approximately same in the magnitude indicating that the pure thermal contributions are much smaller than the pure vacuum results. We also note that for a given bare coupling \( \beta_0 \), both the thermal +
vacuum and pure vacuum expectation value enhances by the same factor on adding tadpole correction factors in the calculation of the covariant derivative. In Fig. 6.11(c), we show the expectation value of the operator $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F_3^i D_4^i F_3^i - F_4^i D_4^i F_4^i] \rangle$ as a function of $\beta_0$. Here as well, the vacuum contributions are most dominant. We also computed the expectation value of $g_0^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F_3^i F_3^i - F_4^i F_4^i] \rangle$, $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F_3^i D_4^2 F_3^i - F_4^i D_4^2 F_4^i] \rangle$ and $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F_3^i D_4^2 F_3^i - F_4^i D_4^2 F_4^i] \rangle$ for $n_\tau = 6$ (Fig. 6.12) and $n_\tau = 8$ (Fig. 6.13), and have observed trend similar to the case of $n_\tau = 4$.

![Graphs showing FF correlators in unquenched SU(3) plasma for lattice size $n_\tau=4$, $n_s=16$.](image)

(a) Thermal + FF (red color) and pure vacuum (blue color) expectation value of $g_0^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F_3^i F_3^i - F_4^i F_4^i] \rangle$. (b) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F_3^i D_4^2 F_3^i - F_4^i D_4^2 F_4^i] \rangle$ in absence of tadpole corrections for the links $U_\mu$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in presence of tadpole factors. (c) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F_3^i D_4^2 F_3^i - F_4^i D_4^2 F_4^i] \rangle$ in absence of tadpole corrections for the links $U_\mu$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in the presence of the tadpole factors.

### 6.6.2 Scale setting for 2+1 flavor SU(3) lattices

To understand the behavior of these operators in terms of physical quantities, we need to relate the bare coupling constant with the lattice spacing. For the action involving the fermions, the lattice spacing is determined using either scale parameter $r_0$ or $r_1$, defined in
terms of the static heavy quark and anti-quark potential as

\[ r^2 \frac{dV(r)}{dr} \bigg|_{r=r_0} = 1.65, \quad r^2 \frac{dV(r)}{dr} \bigg|_{r=r_1} = 1.0. \quad (6.44) \]

The MILC collaboration has performed a more precise determination of the scale \( r_1 = 0.3106(8)(18)(4) \) fm using pion decay constant \( f_\pi \) \[144\]. This was in agreement with previous value obtained by HPQCD collaboration \( r_1 = 0.3091(44) \) fm using bottomium splitting, \( r_1 = 0.3148(28)(5) \) fm using the decay constant \( (f_{s\bar{s}}) \) of the fictitious pseudoscalar \( s\bar{s} \) meson, \( r_1 = 0.3157(53) \) of \( D_s \) and \( \eta_c \) mesons \[145\]. To set the scale using \( r_0 \), one can use estimates \( r_0 = 0.462(11)(4) \) fm by the MILC collaboration \[146\] and \( r_0 = 0.469(7) \) fm by the HPQCD collaboration \[147\].

In order use estimates of \( r_0 \) or \( r_1 \), we need to calculate the derivative of the potential
Figure 6.13: FF correlators in unquenched SU(3) plasma for lattice size $n_s=8$, $n_a=32$. (a) Thermal + Vacuum (red color) and pure vacuum (blue color) expectation value of $g_0^2 a^4 \sum_{i=1,2} \langle \text{Tr}[F^{3i} F^{3i} - F^{4i} F^{4i}] \rangle$. (b) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^6 \sum_{i=1,2} \langle \text{Tr}[F^{3i} D_i^2 F^{3i} - F^{4i} D_i^2 F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_\mu$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in presence of tadpole factors. (c) Thermal + Vacuum (black color) and pure vacuum (green color) expectation value of $g_0^2 a^8 \sum_{i=1,2} \langle \text{Tr}[F^{3i} D_i^4 F^{3i} - F^{4i} D_i^4 F^{4i}] \rangle$ in absence of tadpole corrections for the links $U_\mu$ in the covariant derivative. The curves in red color and blue color represents the expectation value of the correlator in the presence of the tadpole factors.

from our numerical data. The static potential can parametrized by

$$V(r) = A + \frac{B}{r} + \sigma r,$$  \hspace{1cm} (6.45)

where $A$, $B$, $C$, are fit parameters and $r$ is the distance between the quark and anti-quark. The term $B/r$ represents Coulomb potential at short distance, whereas $\sigma r$ represents linear potential at long distances. Now, we employ the condition given in Eq. (6.44),

$$r_1^2 \frac{dV(r)}{dr} \bigg|_{r=r_1} = -B + \sigma r_1^2 = 1.0$$

$$\Rightarrow r_1 = \sqrt{\frac{1.0 + B}{\sigma a^2}}$$

(6.46)

The ratio $r_1/a$ is completely determined once we know the parameters $B$ and $\sigma a^2$. These are determined from fits to the numerical data obtained for $a V(an)$ as a function of $n$, where
Using the static potential, we write the fit function as

$$aV(an) = Aa + \frac{B}{n} + \sigma a^2 n,$$

(6.47)

where $Aa$, $B$, $\sigma a^2$ are fit parameters.

Numerically, the static potential $aV(an)$ is determined either by computing the Wilson line correlator or planar Wilson loop. The MILC and TUMQCD collaboration uses a Wilson line correlator in Coulomb gauge to compute the static potential [148]. Here, we discuss the calculation based on the planar Wilson loop method. In this method, $aV(an)$ obtained by computing the vacuum expectation value of planar Wilson loops (rectangular contour) of size $r \times t$. The spatial distance $r$ and Euclidean time $t$ are given as $r = na$ and $t = n_\tau a$, respectively. For lattices $n_\tau \gg n_s$, one can write the vacuum expectation value of the Wilson's planar loop in terms of static potential as

$$\langle W_{r \times t} \rangle \approx c \exp[-tV(r)] = c \exp[-n_\tau aV(na)],$$

(6.48)

where the higher-order corrections in the exponential are suppressed in the limit of $an_\tau \to \infty$.

For a given value of bare coupling $\beta_0$, the fit is carried out in two steps. In first step, we fix $n$ and determine the $\langle W_{r \times t} \rangle$ on the lattice for different $n_\tau$. This numerical data is then fit using Eq. 6.48 to extract the value of $c$ and $aV(an)$. The second step is to repeat this procedure for different values of $n$, which gives us a set of numerical data for $aV(an)$ as a function $n$. Finally, one uses this numerical data to fit Eq. 6.47 while treating $Aa$, $B$ and $\sigma a^2$ as fit parameters. Once we know the value of fit parameters $B$ and $\sigma a^2$, we plug them into Eq. 6.46 to obtain the scale $r_1/a$. Using the known value of the $r_1$ and the ratio $r_1/a$, one can determine the lattice spacing $a$. This procedure can be repeated for different values of bare coupling $\beta_0$.

The scale setting based on the Wilson line correlator has been systematically carried out for the “HISQ + tree-level Symazik gauge action” by the HotQCD Collaboration [13].
TUMQCD collaboration [14, 148]. We have used their scale setting results in our study as the gauge configurations we generated for "HISQ+ tree level Symanizk gauge action" were for identical input parameters. The scale setting results and input parameters used in this thesis are listed in Table-III ($n = 8$), Table-IV ($n = 6$) and Table-V ($n = 4$) in Ref. [14].

### 6.6.3 Temperature dependence of vacuum subtracted operators

We present the vacuum subtracted expectation value of FF correlators as a function of temperature in Fig. 6.14(a), 6.14(b) and 6.14(c) for $n = 4, 6$ and 8, respectively. In all three plots, the red points represent the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] \rangle$ scaled by $T^4$ to make it dimensionless. The points in blue color represents the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i}D_z^2F^{3i} - F^{4i}D_z^2F^{4i}] \rangle$ scaled by $T^4(q^-)^2$ to make it dimensionless. The factor $(q^-)^2$ is used because a quadratic power of the hard scale $q^-$ appears in the denominator of the second-order covariant derivative FF correlator term. This allows us to estimate relative strength between the operators at $n = 0$ and $n = 2$ in the $\hat{q}$ series (Eq. 6.14). The points in black color represents the vacuum subtracted expectation value of $\sum_{i=1,2} \langle \text{Tr}[F^{3i}D_z^4F^{3i} - F^{4i}D_z^4F^{4i}] \rangle$ scaled by $T^4(q^-)^4$. As quartic power of $q^-$ appears in the FF correlators at $n = 4$ in the $\hat{q}$ series, the operator is scaled by 4th-power of $q^-$. The hard quark light-cone energy $q^-$ is set to 100 GeV.

Our calculations show that the operator $\sum_{i=1,2} \langle \text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] \rangle / T^4$ (red color) is dominant among all three operators. The FF correlator term with the second-order covariant derivative is suppressed by a factor of $10^3$, whereas the term with the fourth-order covariant derivative is suppressed by a factor of $10^6$ relative to the operator in red color. Overall, we observe that the correlator $\langle \text{Tr}[F^{3i}F^{3i} - F^{4i}F^{4i}] \rangle$ (red curve) shows a rapid transition near the critical temperature $T \in (150, 200)$ MeV and is dominant at high temperature compared to rest of the operators. The large error bars in the operators with covariant derivative at $n = 8$ is mainly due to poor statistics and requires generating more gauge configurations.
are similar to operators in trace anomaly, the lattice operator $\text{Tr}[F^3_i F^3_i - F^4_i F^4_i]/T^4$ (red color), $\sum_i \langle \text{Tr}[F^3_i D^2 D^2_i F^3_i - F^4_i D^2 D^2_i F^4_i]/(T^4(q^-)^2) \rangle$ (blue color) and $\sum_i \langle \text{Tr}[F^3_i D^2 D^3_i - F^4_i D^2 D^3_i F^4_i]/(T^4(q^-)^4) \rangle$ (black color) in 2+1 flavor SU(3) plasma. We used $q^-$ as 100 GeV. The links in the covariant derivative are tadpole improved. (a) The real part of FF correlators for $n\tau = 4$ and $n_s = 16$. (b) The real part of FF correlators for $n\tau = 6$ and $n_s = 24$. (c) The real part of FF correlators for $n\tau = 8$ and $n_s = 32$.

6.7 Renormalization factor for FF correlators

In general, the operators computed on the lattice require a renormalization in order to be converted into meaningful physical quantities. In our case, the lattice operators needed to be renormalized are vacuum subtracted operators: $\sum_{i=1,2} \langle \text{Tr}[F^3_i F^3_i - F^4_i F^4_i] \rangle$, $\sum_{i=1,2} \langle \text{Tr}[F^3_i D^2 D^3_i F^3_i - F^4_i D^2 D^3_i F^4_i] \rangle$ and $\sum_{i=1,2} \langle \text{Tr}[F^3_i D^4 D^3_i F^3_i - F^4_i D^4 D^3_i F^4_i] \rangle$. Since each $F_{\mu\nu}$'s are built up from the product of at least four links, and each link requires the multiplicative renormalization for its self-energy divergence in any expectation value.

To determine the proper renormalization factor, we draw a connection with operators that appear in the calculation of the equation of state (EOS). We know that the trace anomaly ($\langle -3p \rangle/T^4$) is computed using the vacuum subtracted expectation value of the action density ($-1/4)F_{\mu\nu}F^{\mu\nu}$. In this calculation, lattice beta function $R_{\beta_0} = -ad\beta_0/da$ appear as a multiplicative renormalization factor [13]. Since, the FF operators in our case are similar to operators in trace anomaly, the lattice operator $\text{Tr} [F^2_{3i} - F^2_{4i}]$ must have $R_{\beta_0}$
as the multiplicative renormalization factor and hence, we scale

\[
\sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 F_{3i}^3 - F_{4i}^4 F_{4i}^4] \rangle \rightarrow R_{\beta_0} \sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 F_{3i}^3 - F_{4i}^4 F_{4i}^4] \rangle
\]

\[
\sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 D_z^2 F_{3i}^3 - F_{4i}^4 D_z^2 F_{4i}^4] \rangle \rightarrow R_{\beta_0} \sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 D_z^2 F_{3i}^3 - F_{4i}^4 D_z^2 F_{4i}^4] \rangle
\]

\[
\sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 D_z^4 F_{3i}^3 - F_{4i}^4 D_z^4 F_{4i}^4] \rangle \rightarrow R_{\beta_0} \sum_{i=1,2} \langle \text{Tr}[F_{3i}^3 D_z^4 F_{3i}^3 - F_{4i}^4 D_z^4 F_{4i}^4] \rangle
\]

(6.49)

Thus, in the final calculation of \( \hat{q} \) (Eq. 6.14), we would employ FF operators scaled by factor \( R_{\beta_0} \) as shown in Eq. 6.49.

\[
\beta_0 = \frac{6}{g_0^2}
\]

To determine \( R_{\beta_0} = -ad\beta_0/\, da \) for the case of pure SU(3) gauge, we employ Eq. 6.37 and compute derivative of \( \beta_0 \) with respect to lattice spacing \( a \). We present the extracted \( R_{\beta_0} \) for pure SU(3) gauge theory employing Wilson’s action in Fig. 6.15(b). We observe that as the coupling \( g_0 \) decreases, the \( R_{\beta_0} \) increases and rises from 0.4 to 0.8. In Fig. 6.15(a), we present the lattice beta function \( R_{\beta_0} \) for the case of (2+1)-flavor QCD using “HISQ + tree level Symanzik gauge action” computed by the HOTQCD collaboration [13]. We observe
that $R_{30} \in [1.0, 1.15]$.

### 6.8 Results and Discussions

In this section, we present our results of the transport coefficient $\hat{q}$ for the case of (2+1)-flavor QCD and pure SU(3) gauge plasma using the setup described in previous sections. To compute $\hat{q}$ using Eq. 6.14, we need to evaluate perturbative $\alpha_s$ that represents the coupling between the hard quark and the transverse gluon. We evaluate $\alpha_s$ at the scale $\mu^2 = (\pi/a)^2 = (\pi T n_\tau)^2$ for a given temperature $T$ and lattice size $n_\tau$. This scale is the same as the scale at which our FF correlators are computed on the lattice. The light-cone momentum (energy) $q^{-}$ of the hard quark traversing the plasma was set to 100 GeV.

Now, we present our final result of $\hat{q}$ in Fig. 6.16 computed on quenched SU(3) and unquenched SU(3) lattices. The solid symbol represents $\hat{q}/T^3$ (dimensionless) for full QCD plasma calculated using “HISQ + tree level Symanzik gauge action” with (2+1)-flavor of quarks on lattice sizes $n_\tau = 4$ (red circle), $n_\tau = 6$ (blue triangle) and $n_\tau = 8$ (black star). The temperature range is covered from $150 < T < 860$ MeV to facilitate a realistic comparison with phenomenology based extracted $\hat{q}$ for QCD plasma produced in RHIC and LHC collision energies. At high temperatures, our unquenched lattice results constrains $\hat{q}/T^3 \sim 2.5-3.5$ and $\hat{q}$ seems to scale with $T^3$. The open symbol in Fig. 6.16 represents $\hat{q}/T^3$ (dimensionless) for pure gluon plasma computed using Wilson’s gauge action on lattice sizes $n_\tau = 4$ (red circle), $n_\tau = 6$ (blue triangle) and $n_\tau = 8$ (black star). At high temperatures, our quenched lattice result constrains $\hat{q}/T^3 \sim 1.5-2.5$ and $\hat{q}$ seems to scale with $T^3$.

For the case of unquenched plasma, the $\hat{q}/T^3$ does not show a clear scaling behavior as one goes from the coarser to the finer lattice ($n_\tau = 4 \rightarrow n_\tau = 8$). This is mainly because of the improved action employed in the calculation, which has discretization error $O(a^4) + O(g^2 a^2)$. However, the lattice results for quenched plasma do show a clear scaling behavior as one goes from the coarser to the finer lattice ($n_\tau = 4 \rightarrow n_\tau = 8$). This is due to the fact that we employed Wilson’s gauge action in the calculation, which has discretization error $O(a^2)$. In low temperature region $T \in (250, 350)$ MeV [pure SU(3)] and $T \in (150, 250)$ MeV [(2+1)-
flavor QCD], we note that $\hat{q}/T^3$ exhibits a rapid increase in the magnitude. The qualitative behavior $\hat{q}/T^3$ is similar to the temperature dependence of the entropy density (Fig. 1.1). We also note that our lattice extracted $\hat{q}$ does not show any signature of log-like behaviour as one see in the hard-thermal-loop based $\hat{q}$ formula, i.e. $\hat{q} \propto T^3 \log(E/T)$ [9,15,125].

In Fig. 6.17 we show a comparison of our lattice extracted $\hat{q}$ with the phenomenology based extraction of $\hat{q}$ carried out by the JET and JETSCAPE collaborations [9,15]. We see a reasonable agreement with the JET and JETSCAPE collaborations results. We also note that $\hat{q}/T^3$ has a weak temperature dependence at high temperature, a feature common to both lattice and phenomenology based results shown in the same plot.

![Graph showing $\hat{q}/T^3$ vs. $T$ (MeV)](image)

Figure 6.16: Temperature dependence of $\hat{q}$ for full qcd plasma and pure gluon plasma at lattice sizes: $4 \times 16^3$, $6 \times 24^3$ and $8 \times 32^3$. The light-cone momentum (energy) $q^-$ of the hard quark traversing the plasma was set to be 100 GeV.

In this chapter, we carried out a lattice QCD based study of the jet quenching parameter
\( \hat{q} \), which is a leading coefficient that controls the jet energy-loss in the medium. In this work, we have established a first-principles framework of \( \hat{q} \), applicable to 4D hot quark-gluon plasma as well as pure gluon plasma. We considered a leading-order process where the hard quark propagates through a section of plasma at temperature \( T \), while exchanging a transverse gluon with the plasma. In order to express \( \hat{q} \) in terms of local operators, we defined a generalized coefficient \( \hat{Q}(q^+) \) and did an analytic continuation in \( q^+ \) complex-plane. Next, we showed how this generalized coefficient \( \hat{Q}(q^+) \) is connected to the physical \( \hat{q} \) when studied in the region where \( |q^+| \ll q^- \). We also found that this object in the region \( q^+ \sim -q^- \), can be expressed in terms of a series of local operators. We used the method of dispersion relations to relate the two regions. Within the framework of lattice gauge theory, we employed the clover-definition of \( F_{\mu\nu} \) to compute FF correlators on quenched SU(3) plasma and unquenched SU(3) plasma. The FF operators on a quenched SU(3) plasma were computed for different lattice sizes using Wilson’s gauge action, and our results displayed a
good scaling behavior.

Our quenched lattice result constrains $\hat{q}/T^3 \sim 1.5$-2.5 at high temperatures. The lattice formulation of $\hat{q}$ discussed in this paper represent a first successful attempt towards realizing a first principle formulation of $\hat{q}$. We also computed the local FF operators on the unquenched SU(3) lattices using “HISQ + tree-level Symanzik gauge action” with two degenerate flavors of light quark and one heavy strange quark. Our unquenched lattice results constrain $\hat{q}/T^3 \sim 2.5$-3.5 at high temperatures. We would like to emphasize that the expression of $\hat{q}$ appearing in the Eq. 6.14 is valid for both pure gluon plasma and the quark-gluon plasma. Our lattice results are consistent with the JET and JETSCAPE collaborations results within their uncertainty band. The qualitative behavior of the temperature dependence of $\hat{q}/T^3$ from lattice is similar to the temperature dependence of the entropy density. We also note that our lattice extracted $\hat{q}$ does not show any signature of a log-like behavior as one sees in the hard-thermal-loop based $\hat{q}$ formula, i.e., $\hat{q} \propto T^3 \log(E/T)$.

For future attempts, we will include the contributions from the medium-induced radiative splitting and take a closer look at the renormalization aspects of lattice operators. To improve the numerical accuracy, we would like to increase the statistics for $n_\tau = 8$ gauge configurations (full QCD case). Moreover, to identify scaling behavior and achieve better control of the continuum limit, we would extend the calculation to finer lattice sizes $n_\tau = 10$ and $n_\tau = 12$. These extensions would allow us to perform a continuum extrapolation of $\hat{q}$. In this chapter, we studied the transport coefficient $\hat{q}$ for single parton traversing the QGP. In the subsequent chapter, we shall also focus on understanding the scale dependence of the jet itself.
CHAPTER 7  JET QUENCHING IN A MULTI-STAGE MONTE CARLO APPROACH

In the preceding chapter, we studied the transport coefficient $\hat{q}$ that is responsible for the modification of the single hard parton. In this chapter, we shall extend the study beyond $\hat{q}$ and focus on understanding multiple scales and regions involved in the jet energy-loss, as depicted in Fig. 2.3. A complete description of jet modification in QGP must address the role and interplay of the physics at each of these scales and their effect on leading hadrons and jet observables. In this chapter, we present a jet quenching model within a unified multi-stage framework and demonstrate for the first time a simultaneous description of leading hadron and inclusive jet observables, which spans multiple centralities and collision energies. In this approach, we shall setup an effective parton evolution that includes a high-virtuality radiation dominated energy loss phase, followed by a low-virtuality scattering dominated energy loss phase. Measurements of jet and charged-hadron $R_{AA}$ set strong constraints on the jet quenching model. Since jet observables are sensitive to the modification of the soft parton in addition to the hard parton, a jet-medium response is also included through a weakly-coupled transport description.

7.1 JETSCAPE framework

Ultra-relativistic nucleus-nucleus collisions performed at the Relativistic Heavy-Ion Collider (RHIC) and Large Hadron Collider (LHC) produce an exotic state of deconfined matter that undergoes different stages, namely: initial state hard scattering, expansion of deconfined quark-gluonic matter, jet energy loss in the medium, and hadronization. A unified framework that implements all stages of a heavy-ion collision is required to gain a comprehensive understanding of the QGP and explore new physics. Jet Energy-loss Tomography with a Statistically and Computationally Advanced Program Envelope (JETSCAPE) is a state-of-the-art simulation framework with capabilities to accommodate physics of each stage of the heavy-ion collision in a modular form \[16,45,149\].

This simulation framework supports incorporation of a wide variety of existing software
such as TRENTO (2+1)-D and (3+1)-D code package \[150\] to model the initial state of the nuclei, Pythia8 based initial state hard scattering, MUSIC \[31\] to simulate the viscous hydrodynamic expansion of the QGP, MATTER/LBT/MARTINI/ADS-CFT \[151\]–\[157\] based energy loss routines, Pythia8 based string fragmentation \[16\]–\[45\], Liquefier module to create jet source terms energy deposition in the medium \[158\]–\[159\], SMASH for hadronic cascade \[160\] etc. We demonstrate that a multi-stage jet quenching model gives a simultaneous description of the jet and hadron observables at multiple centralities and collision energies. Results presented in this chapter are from simulations performed using the JETSCAPE code package version 2.2 within the JETSCAPE collaboration \[17\]–\[46\].

### 7.2 Multi-stage jet energy loss within JETSCAPE framework

It has been widely accepted that the evolution of jets through deconfined QCD matter is a multi-scale problem. To incorporate this property within the JETSCAPE framework, we set up an effective parton evolution in which we incorporated information of the space-time evolution of the medium on parton energy loss during the high-virtuality, radiation dominated portion of the shower using MATTER, followed by a simulation of the low-virtuality, scattering dominated portion with LBT. The switching between energy-loss stages is performed at a parton-by-parton level depending on local quantities such as local energy density in the medium, off-shellness and energy of the parton.

MATTER \[151\]–\[161\] is a virtuality-ordered Monte Carlo event generator that simulates the evolution of partons at high energy (\(E\)) and high-virtuality (off-shellness) \(Q^2 \gg \sqrt{qE}\), where \(q\) is the transport coefficient that controls transverse broadening, and \(Q^2 \geq 1 \text{ GeV}^2\). Based on the Higher-Twist formalism, the probability of a parton splitting is computed by sampling the medium modified Sudakov form factor which includes contributions from the
vacuum and medium-induced splitting functions. The Sudakov form factor is given as

$$
\Delta(t, t_0) = \exp \left[ - \int_{t_0}^{t} \frac{dQ^2}{Q^2} \frac{\alpha_s(Q^2)}{2\pi} \int_{t_0/t}^{1} dz P(z) \right] \\
\times \left\{ 1 + \int_{0}^{\xi_{\text{max}}} d\xi^- \frac{\hat{q}(r + \xi)}{Q^2 z(1 - z)} \phi(Q^2, q^-, \xi^-) \right\},
$$

(7.1)

where $\phi$ represents the phase factors that depends on the hard parton’s energy $q^-$, location $\xi^-$ and virtuality $Q$. The function $P(y)$ represents the vacuum splitting function, $\hat{q}$ is the transport coefficient that controls the transverse broadening, $\xi_{\text{max}}$ represents the maximum length ($\sim 1.3\tau^-_f$) over which the splitting is sampled, $\tau^-_f = 2q^-/Q^2$ is the mean light-cone formation time of the given parton. The momentum fraction $z$ of the split can be computed by sampling the splitting function $P(z)$.

To determine the transverse momentum of the daugthers in the split, we compute the difference in the invariant mass between the parent parton and the daugthers. This process is repeated until the virtuality of the parton reaches a predetermined value of $Q^2_0$, usually taken to be 1-3 GeV$^2$. We used a hard thermal loop formulation for $\hat{q}$ [125]. The medium response is included through a weakly-coupled description of the medium in terms of thermal partons, where the propagation of the medium parton kicked out by the jet parton (“recoil”) is described by a kinetic theory-based approach.

LBT [153,154,162] is also a Monte Carlo event generator based on the linear Boltzmann equation which simulates in-medium energy loss of high-energy, low-virtuality partons. The model includes both the elastic $2 \rightarrow 2$ scattering processes and inelastic $2 \rightarrow 2 + n$ scattering with multiple gluon radiation. The rate of the elastic scattering of the hard parton with the thermal parton from medium is computed using leading-order matrix elements for all possible scattering channels “$12 \rightarrow 34$” between the hard parton and thermal parton sampled from the medium. In the case of an inelastic process, the rate is computed using the medium-
induced gluon spectrum,

$$\Gamma^{\text{inel}} = \int dx dk_\perp^2 \frac{dN_g}{dx dk_\perp^2 dt}, \quad (7.2)$$

where \( x \) is momentum fraction of the emitted gluon with respect to its parent and \( k_\perp \) is the transverse momentum of the emitted gluon transverse to the direction of the parent. In Eq. 7.2, \( \frac{dN_g}{dx dk_\perp^2 dt} \) represents the differential spectrum of the radiated gluon given as

$$\frac{dN_g}{dx dk_\perp^2 dt} = \frac{2\alpha_s C_A P(x)k_\perp^4}{\pi(k_\perp^2 + x^2m^2)^4} \hat{q} \sin^2 \left( \frac{t - t_i}{2\tau_f} \right) \quad (7.3)$$

where \( C_A = N_c \) is color factor, \( P(x) \) is the splitting function, \( t_i \) is the initial location of the hard parton, \( t \) is the location where the split happens and \( \tau_f \) is the formation time of the radiated gluon.

The probabilities of these scattering processes are employed to simulate the evolution of the jet shower, recoil partons, and radiated gluons due to their scattering with thermal partons in the medium. The thermal partons that are scattered out of the medium and become part of the jet are called “recoiled partons”. In this process, the thermal partons sampled from the medium are recorded separately in order to keep track of the energy-momentum injected into the jet from the medium. In final calculations, one subtracts the energy-momentum injected into the jet from the medium to compare with the experimental results. The hadronization of the “jet+recoil” partons and parton sampled from the medium is carried out separately.

### 7.3 JETSCAPE pp19 tune

To simulate proton-proton collisions, we use PYTHIA 8.230 in JETSCAPE to generate the initial state hard scattering with the underlying events. The parameters in the PYTHIA 8.230 are set by the default tune “Monash 2013” with proton PDF NNPDF2.3 LO. The underlying events are accounted for by including multi-parton interactions (MPIs) and initial state radiations (ISRs). In this setup, within the PYTHIA8, we turn off the final state radiations (FSR) and hadronization. To simulate the final state radiation for the partons
obtain from initial state scattering, we employ MATTER event generator \[151, 161\], which has capabilities to generate vacuum as well as in-medium parton shower. MATTER is primarily based on the DGLAP equation \[53, 54\] and hence, the parton shower generated is virtuality ordered. This evolves partons from their initial virtuality to the minimum virtuality \(Q_{\text{min}} = 1\) GeV. Once all partons achieve the minimum virtuality, a PYTHIA8 based string fragmentation is employed for hadronization.

In the JETSCAPE framework, two popular hadronization methods are “Colored hadronization” and “Colorless hadronization”. The label “colored” means that the color information for partons in the MATTER parton shower is preserved and utilized in the PYTHIA8 based string fragmentation. This can be achieved in the case of a vacuum shower (p-p), but not when the medium is present. In the presence of the medium, the color is exchanged in in-medium scattering processes, and hence color coherence can be lost in the parton shower. To circumvent this issue, the framework has an alternative hadronization module called “colorless hadronization”. In this method, the original color information in the final state partons is ignored and one re-assign color to each parton after establishing the strings. In the colored hadronization, we need one external parton for each shower initiating parton. However, in the case of colorless hadronization, we only need one external parton for the entire shower to make the shower color singlet. The color assignment is done in the large-\(N_c\) limit.

The setup for to simulate p-p collisions has two free parameters: \(Q_{\text{ini}}\) and \(\Lambda_{\text{QCD}}\). The parameter \(Q_{\text{ini}}\) represents the initial virtuality of the parton obtained from PYTHIA8 initial state hard scattering. We adjust these two parameters to obtain a good description of the inclusive jet cross section at midrapidity. The best fit is obtained when \(Q_{\text{ini}} = p_T/2\) and \(\Lambda_{\text{QCD}} = 200\) GeV. This choice of the free parameters and the setup described above establishes the JETSCAPE pp19 tune \[16\]. In Fig. 7.1(a), we present a comparison of inclusive jet cross section obtain using colored and colorless hadronization with the experimental data. The ratio is taken with respect to the result obtained from the default PYTHIA8. The jets are defined using anti-\(k_T\) algorithm \[163\] within the FASTJET package \[164, 165\], with
kinematic cuts consistent with experiments. The two JETSCAPE results give compatible results and are typically within the 10% deviation from the experimental data. However, the default PYTHIA8 results show a deviation of $\sim 20\%$ from the experimental data. In Fig. 7.1(b), we present inclusive jet cross section two collision energies and three different jet radii. Results are consistent within the uncertainties of the experimental data.

![Graph](image)

Figure 7.1: Comparison of JETSCAPE PP19 tune’s results for inclusive jets with the experimental data [16]. (a) Ratio of inclusive jet cross-sections as a function of jet $p_T$ for cone size $R = 0.7$. The ratio is taken w.r.t. to the default PYTHIA result. (b) Inclusive jet cross section at midrapidity compared to LHC measurements at $\sqrt{s} = 2.76$ TeV and 7 TeV.

### 7.4 Simulation of PbPb events at LHC collision energies

Simulation of PbPb collision events at 5.02A TeV is done by using fluctuating initial state conditions evolved hydrodynamically within the JETSCAPE framework. TRENTO [150] + PYTHIA is used to simulate the initial state hard scattering. The medium profiles are generated using (2+1)-D VISHNU [166] with fluctuating TRENTO [150] initial conditions. The input parameters in the soft-sector such as shear viscosity to entropy ratio $\eta/s = 0.8$ were tuned to obtain a good description of the soft hadronic spectra and elliptic flow observables at RHIC and LHC collision energies. The virtuality-ordered shower is generated using an in-medium MATTER generator, which evolves partons to a lower virtuality $Q_0$ (switching virtuality). Then, these partons are passed to a small-virtuality energy-loss stage, LBT.
The jet quenching start time was set to $\tau_0 = 0.6$ fm/c. The jet quenching parameter $\hat{q}$ was scaled as $\hat{q} = \hat{q}_{\text{local}} \cdot p^\mu u_\mu/p^0$. It is evaluated using the temperature, entropy, and flow velocity obtained from the hydrodynamical calculations. In both energy-loss models, we used a hard thermal loop formulation for $\hat{q}$ [125]. We set $\hat{q} = 0$, for the cases when the parton is outside the QGP regime, i.e. $\tau < 0.6$ fm and local temperature $T < 165$ MeV. Finally, the jet partons are hadronized using a PYTHIA based string fragmentation called colorless hadronization.

7.5 Results: Inclusive jets and leading hadron observables

In this section, we present results for inclusive jets and leading hadron observables for pp at $\sqrt{s} = 5.02$ TeV using the JETSCAPE pp19 tune. We also constrain the in-medium free parameters: the jet-medium coupling parameter $\alpha_s$ and the switching virtuality $Q_0$ for MATTER+LBT as a multi-stage jet energy loss model. The Fig. 7.2 displays a ratio of inclusive jet cross-sections (left) and charged-hadron yields (right) for p-p collisions at $\sqrt{s} = 5.02$ TeV. In the JETSCAPE pp19 tune, we employed colorless hadronization. Overall, the JETSCAPE results are compatible with the experimental data (within 10%). Results from PYTHIA tend to be similar to JETSCAPE for the case of the charged-hadron yield, but for jets show discrepancies of order $\lesssim 25\%$. Both observables provide a good baseline for their counterparts in nuclear collisions.

In Fig. 7.3, we show inclusive jet $R_{AA}$ (left) and charged-hadron $R_{AA}$ (right) in most central 5.02A TeV PbPb collisions (0-10\%) for switching virtualities $Q_0 = 1, 2, 3$ GeV and the jet-medium coupling parameter $\alpha_s = 0.25$. Increasing $Q_0$ from 1 to 3 GeV increases the effective length of LBT based energy-loss. Since the partons in the LBT stage are close to on-shell ($Q_0 \sim [1,3]$ GeV, $E \sim p_T$), the partons at low-$p_T$ see significant energy loss effects. Due to this, increasing $Q_0$ from 1 to 3 GeV suppresses the low-$p_T$ region of the charged-hadron $R_{AA}$ spectrum. This leads to suppression of the jet $R_{AA}$ at all jet $p_T$’s. The parameter set $Q_0 = 2$ GeV and $\alpha_s = 0.25$ provides the best simultaneous description of the jet and hadron $R_{AA}$ data. We observe a $\sim 20\%$ deviation at high $p_T$ in the charged-hadron
Figure 7.2: Comparison of JETSCAPE PP19 tune’s results for inclusive jets and charged-hadrons with the experimental data and the default PYTHIA at 5.02 TeV \cite{17}. The ratio is taken w.r.t. to the default PYTHIA result. (a) Ratio of inclusive jet cross-section as a function of jet $p_T$ for cone size $R = 0.4$ and $|y_{\text{jet}}| < 0.3$. (b) Ratio of charged-hadron yield as a function of charged-hadron $p_T$.

$R_{AA}$ that could be due to the absence of any scale dependence (hard parton’s off-shellness) in $\hat{q}$ \cite{40}.

Figure 7.3: Comparison of the nuclear modification factor for inclusive jets and charged-hadrons obtained using the multi-stage energy loss approach (MATTER+LBT) within the JETSCAPE framework, with the experimental data for most central 5.02A TeV collisions (0-10%). Results are shown for a switching virtuality parameter $Q_0 = 1$, 2, and 3 GeV \cite{17}. (a) Jet $R_{AA}$ as a function of jet $p_T$ for cone size $R = 0.4$. (b) Charged-hadron $R_{AA}$ as a function of charged-hadron $p_T$.

In Fig. 7.4 we show inclusive jet $R_{AA}$ (left), charged-hadron $R_{AA}$ (center) and azimuthal
Figure 7.4: Comparison of inclusive jet and charged-hadron nuclear modification factor, and azimuthal anisotropy $v_2$ obtained using the multi-stage energy loss approach (MATTER+LBT) within the JETSCAPE framework, with the experimental data for semi-peripheral $5.02 \text{ A TeV}$ collisions. The tuning parameters $Q_0$ and $\alpha_s$ are set by the simultaneous fit of inclusive jet and charged-hadron $R_{AA}$ in the most central $5.02 \text{ A TeV}$ collisions [17]. (a) Jet $R_{AA}$ as a function of jet $p_T$ for cone size $R = 0.4$. (b) Charged-hadron $R_{AA}$ as a function of charged-hadron $p_T$.

Figure 7.5: Comparison of the nuclear modification factor for inclusive jets and charged-hadrons obtained using multi-stage energy loss approach (MATTER+LBT) within the JETSCAPE framework with the experimental data for most-central $2.76 \text{ A TeV}$ collisions. The tuning parameters $Q_0$ and $\alpha_s$ are set by the simultaneous fit of the inclusive jet and charged-hadron $R_{AA}$ in the most central $5.02 \text{ A TeV}$ collisions [17]. (a) Jet $R_{AA}$ as a function of jet $p_T$ for cone size $R = 0.4$. (b) Charged-hadron $R_{AA}$ as a function of charged-hadron $p_T$. 
anisotropy coefficient $\nu_2$ (right) in semi-peripheral 5.02$A$ TeV PbPb collisions for the parameter set ($Q_0$ and $\alpha_s$) extracted from fits to the most central 5.02$A$ collisions inclusive jet $R_{AA}$ and charged-hadron $R_{AA}$ data. The agreement with the experimental measurement is within 10%. In Fig. 7.5 we show inclusive jet $R_{AA}$ (left) and charged-hadron $R_{AA}$ (right) in the most central 2.76$A$ TeV PbPb collisions for the parameter set ($Q_0$ and $\alpha_s$) extracted from fits to the most central collision inclusive jet $R_{AA}$ and charged-hadron $R_{AA}$ data at 5.02$A$ TeV. Results are consistent with the experimental measurements.

7.6 Conclusion

In this chapter, we attempted to explore the interplay between the soft and hard scales involved in the parton energy loss and their effect on a leading hadron and as well as on jet observables. To explore our questions, we utilized a state-of-the-art simulation framework called JETSCAPE, which is developed to study all aspects of relativistic heavy-ion collisions \[16, 17, 45, 46, 149\]. Within the JETSCAPE collaboration, we carried out a comprehensive study of key observables for single hadrons and inclusive jets within a unified multi-stage energy loss framework; we covered multiple centralities and collision energies.

In this work, a multi-stage energy-loss model was constructed by setting up an effective parton evolution in which we incorporated information of the space-time evolution of the medium on parton energy loss during the high-virtuality, radiation dominated portion of the shower using MATTER, followed by a simulation of the low-virtuality, scattering dominated portion with LBT. The free parameters in p+p collisions were fixed by the JETSCAPE PP19 tune. Simulations of Pb+Pb collisions were performed using fluctuating initial state conditions evolved hydrodynamically within the JETSCAPE framework. TRENTO \[150\]+PYTHIA was used to simulate the initial state hard scattering. The medium profiles were generated using (2+1)-D VISHNU \[166\] with fluctuating TRENTO \[150\] initial conditions. The input parameters in the soft-sector such as shear viscosity to entropy ratio $\eta/s = 0.8$ were tuned to obtain a good description of the soft hadronic spectra and elliptic flow observables at RHIC and LHC collision energies. In both energy-loss models,
the transport coefficient $\hat{q}$ was implemented using HTL formula, i.e. $\hat{q} \propto T^3 \log(E/T)$ \cite{125}. Finally, the jet partons were hadronized using a PYTHIA based string fragmentation called colorless hadronization.

A simultaneous fit of the jet $R_{AA}$ and charged-hadron $R_{AA}$ in the most central 5.02$A$ TeV collisions has been carried out to constrain the effective parton energy-loss model. In the virtuality phase-space, the parton energy-loss is dominated by MATTER. The simultaneous fit to hadron-$R_{AA}$ and inclusive jet-$R_{AA}$ data indicate that the parton at virtuality $Q_0^2 = 2$ GeV$^2$ separates the MATTER energy-loss from the LBT energy-loss. The extracted parameters describe charged-hadron and jet $R_{AA}$ in semi-peripheral collisions at multiple collision energies well without further re-tuning the fit parameters. It is demonstrated that our unified approach, based on the multi-stage energy-loss, effectively captures the physics of multi-scale jet quenching in QCD plasma.
CHAPTER 8 SUMMARY AND OUTLOOK

The work carried out in this thesis primarily focuses on exploring the multi-scale dynamics between a hard jet and QGP using theoretical tools from perturbative QCD, lattice QCD, and the JETSCAPE Monte-Carlo event generator. In this thesis, we have addressed the following key research questions:

- What is the underlying structure of the QGP? Is it possible to use the high-$p_T$ hadron observable measurements to extract the substructure of QGP at different resolution scales?

- Can we study transport coefficients controlling the dynamics between the hard parton and QGP using lattice QCD?

- Can one determine the space-time and momentum dependence of the jet energy-loss rigorously and isolate the effects of transport coefficients beyond $\hat{q}$?

In the subsequent sections, we summarize our new work presented in this thesis and provide an outline for future directions.

8.1 Constraints on the inner-structure of QGP using perturbative approach

In chapter 4, we presented our original work in which we explored how the available experimental data on the modification of leading hadrons can be used to extract the inner-structure of the QGP. We focused on the process presented in Fig. 2.2(b) in a regime where the exchanged momenta are at a perturbative scale. We considered a realistic case in which an energetic and highly-virtual hard parton undergoes transverse momentum broadening due to the multiple scatterings before escaping the plasma. Based on the assumption that the multiple scatterings in the plasma are incoherent in high energy and high virtuality phase of the leading parton, we introduced a new concept of the parton distribution function (PDF) for the “QGP degree of freedom” (QGP-DOF) \[40\]. The QGP-DOF represents a struck portion of the QGP (scattering center) enclosing a degree of freedom and is defined as a volume over which the exchanged gluon field is correlated within the plasma.
In chapter 4, we revisited the transport coefficient \( \hat{q} \) which controls the dynamics between the hard parton and QGP, and reformulated it in terms of PDF of QGP-DOF entirely within the framework of perturbative QCD. We described a prescription [A] to compute \( \hat{q} \), in which the exchanged gluon with momentum scales \( k_{\perp}^2 \in [\mu^2/4, 9\mu^2/4] \) were included in the calculations. We also defined another prescription [B] to compute \( \hat{q} \) in which we extended the range of momentum scale of the exchanged gluon to \( k_{\perp}^2 \in [\mu^2, 9\mu^2] \). In turns out that the scale evolution of the QGP-PDF gives rise to energy and scale dependence in the transport coefficient \( \hat{q}(T, E, \mu^2) \). Due to the lack of knowledge of the mass of QGP-DOF, we used estimates from finite temperature field theory and considered a section of the plasma with a mass \((M)\) of 1 GeV. We made an ansatz based on Feynman-Field parametrization and defined the input QGP-PDF at a reference scale \( \mu^2 = 1 \text{ GeV}^2 \). The density of the plasma was parametrized by the local entropy density obtained from (2+1)D viscous hydrodynamics calculation.

To constrain the inner-structure of QGP, we fold this new \( \hat{q}(T, E, \mu^2) \) in the medium-modified fragmentation function within the higher-twist energy-loss formalism. To explore the possible forms of the QGP-PDF, we varied the overall normalization parameter \( \hat{q}_0 \), free parameters in PDF \( a \) and \( b \) to get a good simultaneous description of the hadron-\( R_{AA} \) data at PHENIX (0-10%) and CMS (0-5%) collision energies. The combined \( \chi^2_{DOF} \) at most central RHIC and LHC collisions allowed us to isolate the PDF of the QGP-DOF at a reference scale \( \mu^2 = 1 \text{ GeV}^2 \). The Fig. 4.10(c,d) represents the first successful extraction of inner-structure of QGP in terms of PDFs at a resolution scale \( \mu^2 = 1 \text{ GeV}^2 \). The evolution of the inner-structure of QGP with the scale of the probe can be computed using the DGLAP equation presented in Eq. 4.46.

The best-fit PDF for prescription [A] is shown in blue dashed line; the hadron-\( R_{AA} \) for this choice is presented in Fig. 4.6 which gives a combined \( \chi^2_{DOF} = 4.8 \). Whereas, the best-fit PDF for prescription [B] is shown in blue solid line which give rise to combined \( \chi^2_{DOF} = 5.4 \) (hadron-\( R_{AA} \) shown in Fig. 4.8). The band in Fig. 4.10(c,d) provides an
insight into the nature of entities inside QGP. When QGP is probed at scale $\mu^2 = 1 \text{ GeV}^2$, the quasi-particle inside the QGP appears to have a large sea-like as well as a valence-like momentum distribution with a peak around $x \approx 0.8$. The wide bump near $x \approx 0.8$ supports the calculation for the temperature-dependent plasma with quasi-particles. The large sea contribution can be attributed to the soft particles exchanged within the interacting quasi-particle. For prescription [A], a sea-like distribution produces the best fit to hadron-$R_{AA}$ data, whereas a valence-like distribution works for prescription [B].

Our results indicate that the scale evolution of $\hat{q}$ is indeed a physical effect. To further support our formalism, we also studied the Fourier coefficient $\nu_2$ which characterizes the anisotropy in the azimuthal pattern of the particle distribution. A simultaneous description of hadron-$\nu_2$ was achieved by doing a parameter-free calculation, i.e., the parameters are entirely fixed from the angle-integrated hadron-$R_{AA}$ calculation. We obtained a reasonable description of the experimental data at RHIC and LHC for four different centralities, without having to readjust the free parameters of our formalism (Fig. 4.7 and 4.9).

In addition, the successful extraction of PDF for QGP-DOF, our new formulation of the scale dependence of $\hat{q}$ provides a reasonable explanation to JET collaboration $\hat{q}$ puzzle, i.e., the interaction strength $\hat{q}/T^3$ is higher at RHIC compared to LHC collision energies. For a given plasma temperature, our calculations show that enhancement $\hat{q}/T^3$ at RHIC is purely due to the resolution scale dependence of $\hat{q}$. It was demonstrated that a cusp-like temperature dependence in $\hat{q}/T^3$ is not required for a simultaneous description of hadron-$R_{AA}$ at RHIC and LHC collision energies. Our work presented in chapter 4 has been published in Ref. [40,82].

8.2 Constraints on the temperature dependence of transport coefficient $\hat{q}$ using lattice gauge theory

In chapter 6 we presented our original work in which we studied the process shown in Fig. 2.2(b) by formulating the interaction between the exchanged gluon and the medium in a non-perturbative environment within the framework of lattice QCD. We developed a
first-principles framework to compute the transport coefficient \( \hat{q} \), which characterizes the dynamics between the hard parton and QGP. We considered a leading-order process where the hard quark exchanges a transverse gluon with the plasma held at temperature \( T \). The non-perturbative part is expressed in terms of a non-local (two-point) Field-Strength-Field-Strength (FF) operators.

In order to express \( \hat{q} \) in terms of local operators, we defined a generalized coefficient \( \hat{Q}(q^+, q^-) \) and did an analytic continuation in \( q^+ \) complex-plane, where \( q^- \) represents the light-cone momentum of the hard parton. Next, we showed how this generalized coefficient \( \hat{Q}(q^+) \) is connected to the physical \( \hat{q} \) when studied in the region where \( |q^+| \ll q^- \). We also found that in the region where \( q^+ \sim -q^- \), the object \( \hat{Q}(q^+) \) can be expressed in terms of a series of local operators. We used the method of dispersion relation to relate the two regions. Within the framework of lattice gauge theory, we employed the clover-definition of \( F_{\mu\nu} \) to compute local FF correlators on quenched SU(3) plasma and unquenched SU(3) plasma. The FF operators on a quenched SU(3) plasma were computed for different lattice sizes using Wilson’s gauge action, and our results displayed a good scaling behavior. Our quenched lattice result constrains \( \hat{q}/T^3 \sim 1.5-2.5 \) at high temperatures.

The lattice formulation of \( \hat{q} \) discussed in chapter 6 represents a first successful attempt towards realizing a first principle formulation to understand the dynamics between the hard parton and plasma. For a realistic case, we modeled QGP using “HISQ + tree-level Symanzik gauge action” with two degenerate flavors of light quark and one heavy strange quark action. Our unquenched lattice results constrain \( \hat{q}/T^3 \sim 2.5-3.5 \) at high temperatures. The expression of \( \hat{q} \) derived in Eq. 6.14 is valid for both pure gluon plasma and the quark-gluon plasma. In this study, we demonstrated that our lattice results are consistent with the JET and JETSCAPE collaborations results within their uncertainty band.

The qualitative behavior of the temperature dependence of \( \hat{q}/T^3 \) from lattice is similar to the temperature dependence of the entropy density. We also note that our lattice extracted \( \hat{q} \) does not show any signature of a log-like behavior as one sees in the hard-thermal-loop
based \( \hat{q} \) formula, i.e., \( \hat{q} \propto T^3 \log(E/T) \). We also do not observe any cusp-like behavior. Our results of extracted \( \hat{q} \) eliminate the fit parameter dependence \( \hat{q} \) and hence, can be used to put additional constraints in theoretical jet quenching models. Our results for the case of quenched SU(3) plasma has appeared in Ref. [130,131] and a paper with a detailed discussion of both quenched and unquenched results will soon be submitted for publication.

8.3 Scale dependence of jets, beyond the transport coefficient \( \hat{q} \)

In chapter 7, we focused on studying multiple scales and regions involved in the parton energy-loss, as depicted in Fig. 2.3. In this chapter, we attempted to explore the interplay between soft and hard scales involved in the parton energy loss and their effect on a leading hadron and as well as on jet observables. To explore our questions, we utilized a state-of-the-art simulation framework called JETSCAPE, which is developed to study all aspects of relativistic heavy-ion collisions [16,17,45,46,149]. Within the JETSCAPE collaboration, we carried out a comprehensive study of key observables for single hadrons and inclusive jets within a unified multi-stage energy loss framework; we covered multiple centralities and collision energies.

In this work, a multi-stage energy-loss model was constructed by setting up an effective parton evolution in which we incorporated information of the space-time evolution of the medium on parton energy-loss during the high-virtuality, radiation dominated portion of the shower using MATTER, followed by a simulation of the low-virtuality, scattering dominated portion with LBT. The switching between energy-loss stages is performed at a parton-by-parton level depending on local quantities such as local energy density of the medium, off-shellness and energy of the parton. Since jet observables are sensitive to the modification of the soft parton in addition to the hard parton, we incorprated a weakly coupled description of the jet-medium interaction using recoil, both in MATTER and LBT.

The free parameters in p+p collisions were fixed by the JETSCAPE PP19 tune. Simulations of Pb+Pb collisions were performed using fluctuating initial state conditions evolved hydrodynamically within the JETSCAPE framework. TRENTO [150]+PYTHIA was used
to simulate the initial state hard scattering. The medium profiles were generated using (2+1)-D VISHNU \cite{166} with fluctuating TRENTO \cite{150} initial conditions. The input parameters in the soft-sector such as shear viscosity to entropy ratio $\eta/s = 0.8$ were tuned to obtain a good description of the soft hadronic spectra and elliptic flow observables at RHIC and LHC collision energies. In both energy-loss models, the transport coefficient $\hat{q}$ was implemented using HTL formula, i.e. $\hat{q} \propto T^3 \log(E/T)$ \cite{125}. Finally, the jet partons were hadronized using a PYTHIA based string fragmentation called colorless hadronization. In the virtuality phase-space, the parton energy loss is dominated by MATTER.

The simultaneous fit to hadron-$R_{AA}$ and inclusive jet-$R_{AA}$ data indicate that the parton at virtuality $Q_0^2 = 2$ GeV$^2$ separates the MATTER energy loss from the LBT energy-loss. We conclude from this study that a multi-stage energy-loss formalism is an essential concept for a simultaneous description of leading hadron and jet observables at multiple centralities and collision energies.

8.4 Future directions

The QGP produced in ultra-relativistic nuclear collisions provides an excellent laboratory to test the fundamental theory of strong interaction and bridge the gap between the fundamental QCD theory and the phenomenology in relativistic heavy-ion collisions. The work presented in this thesis serves as a proof-of-principle calculation and can lead us to go in several directions.

In chapter \cite{4} we extracted the inner-structure of QGP in terms of PDF using a single energy-loss approach (virtuality-ordered higher-twist formalism) applicable to description of high-$p_T$ single-hadron observables. In the next step, we would include jet observables as well to further constrain the inner structure of QGP. Since jet observables are sensitive to the modification of both the soft and hard parton, it will require us to borrow the machinery of the multi-scale energy loss approach described in Chapter \cite{7}. The study will provide more stringent tests for our scale-dependent formulation of $\hat{q}$ and help us in a robust extraction of the QGP-PDF. Our formulation of $\hat{q}$ can also be extended and applied to jet modification
in cold nuclear matter relevant to $pA, eA$ (EIC physics) collisions, and test the validity of the formalism.

In chapter 6 we presented the temperature dependence of $\hat{q}$ using the lattice gauge theory. This calculation was based on the single scattering diagram. In the next step, we would perform an NLO calculation by including corrections from the single-scattering induced emission diagram. The lattice calculation of $\hat{q}$ will require us to study proper renormalization factors for the field-strength operators and the new operators that will arise in the inclusion of medium-induced scattering diagram. It will be interesting to explore the scale dependence of $\hat{q}$ using the lattice gauge theory. We shall also extend the calculation to finer lattices $n_T = 10$ and $n_T = 12$ to allow a continuum extrapolation. The extracted temperature dependence of $\hat{q}$ from lattice QCD can be directly used to further reduce the free parameters in the parton energy loss.

In chapter 7 we explored the interplay between soft and hard scales involved in the parton energy loss and their effect on the leading hadron and as well as on the jet observables using the JETSCAPE Monte-Carlo framework. In the next step, we would explore the sensitivity between the different prescriptions of transport coefficient $\hat{q}$ and their effect on single-hadron and jet observables using the multi-stage energy loss approach with the JETSCAPE framework. A wealth of data measured in the current and future RHIC and LHC experiments also allows us to do precision measurements and put strong constraints on the theoretical jet quenching model.

In chapter 4 we had ignored the flavor-dependence while extracting the QGP-PDF. Extracting the flavor dependent QGP-PDF would increase the number of fit parameters in the calculation. This extraction will require a more extensive study, involving both the leading hadrons and jets, and would be well suited for Bayesian statistical methods. Such studies will help us to develop a comprehensive dynamical model of jet quenching for the strongly interacting matter produced in relativistic heavy-ion collisions and elucidate the microscopic structure of the QGP. Moreover, the jet quenching will also be seen in relativistic
Electron-Ion Collider (EIC) $eA$ and $pA$ experiments and will require sophisticated machinery. In this scenario also, the modular nature of the JETSCAPE framework will provide an ideal benchmark tool to explore the physics of the cold nuclear matter. It will give us a window to study the change of the gluon distribution between the cold nuclear matter and QGP.
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ABSTRACT

EXPLORING JET TRANSPORT COEFFICIENTS IN THE QUARK-GLUON PLASMA

by

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The modifications of hard jets play an essential role as multi-scale probes of the properties of the Quark-Gluon Plasma (QGP) produced in high-energy heavy-ion collisions. In this thesis, we explore the interplay between the soft and hard scales involved in the modification of jet partons as they propagate through the QGP. First, we focus on a regime where the exchanged momenta between the hard parton and the medium are at a high enough scale that QCD perturbation theory can be applied. Based on the assumption that the multiple scatterings inside the plasma are incoherent in the high-energy and high-virtuality phase of the parton shower, we introduced a new concept of the Parton Distribution Function (PDF) of a QGP degree of freedom (QGP-DOF). We revisit the transport coefficient \( \hat{q} \), which is a leading parameter that controls the transverse broadening of the hard parton, and reformulate it in terms of the PDF of a QGP-DOF. A model-to-data comparison is performed by constraining the nuclear modification factor \( R_{AA} \) and azimuthal anisotropy coefficient \( \nu_2 \) to reveal the inner-structure of the QGP in terms of a PDF. In addition to this, we focus on the established enhancement in the interaction strength \( \hat{q}/T^3 \) at RHIC relative to LHC collision energies, as discovered by the JET collaboration. The centrality dependence of the high-\( p_T \) hadron nuclear modification factor \( R_{AA} \) and azimuthal anisotropy \( \nu_2 \), at both these collision energies, strongly suggests that the enhancement is not caused by the temperature dependence of \( \hat{q}/T^3 \), but rather by the scale dependence of \( \hat{q} \).
We have also constructed a framework to study the non-perturbative component in the parton energy-loss using lattice QCD. We shall present the first lattice determination of $\hat{q}$ for the pure gluon plasma and a 2+1 flavor QCD plasma. In the end, we also demonstrate the importance of multi-stage energy loss using a Monte Carlo approach. We highlight the role played by the thermal partons in the simultaneous description of the leading hadron and jet observables. This study clearly highlights the effect of transport coefficients beyond $\hat{q}$ in the modification of hard jets. The research presented in this thesis helps us develop a comprehensive model of jet quenching for the strongly interacting matter produced in heavy-ion collisions and elucidates the microscopic structure of the QGP.
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