

Partonic transport model application to heavy flavor

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Introduction

1.1 Nuclear matter under extreme conditions

The quest for the matter and its properties under extreme highly density and temperature has fundamental importance. Understanding nuclear matter and under these conditions help to understand questions from the early dynamics of the universe to the neutron star merger simulation for the gravitational wave studies. It also help to enrich the understanding of the fundamental theory of the strong interaction and basics to the nuclear physics: the Quantum Chromodynamics (QCD).

Quantum Chromodynamics QCD describes the interaction of objects that carries “color” charges. Quarks (fermions) and gluons (bosons) are its elementary degrees of freedom. The QCD Lagrangian (with one flavor of quark) is,

$$\mathcal{L} = \bar{\psi}_i \left(i\gamma_\mu D_{ij}^\mu - m\delta_{ij} \right) \psi_j - \frac{1}{4} G_{\mu\nu}^a G^{\mu\nu,a}, \quad (1.1)$$

where ψ_i the Dirac spinor of the quark field with i the color index.

$$D_{ij}^\mu = \partial^\mu - igT_{ij}^a A^{\mu,a} \quad (1.2)$$

is the covariant derivative, containing the interaction between quark field and the gluon field with coupling strength g . Here T_{ij}^a are the generators of the SU(3) group in the fundamental representation and the generators satisfies the commutation relation,

$$[T^a, T^b] = if^{abc}T^c \quad (1.3)$$

where f^{abc} are known as the structure constants of SU(3). The field tensor of gluon with color a is,

$$G^{\mu\nu,a} = \partial^\mu A^{\nu,a} - \partial^\nu A^{\mu,a} + g f^{abc} A^{\mu,b} A^{\mu,c} \quad (1.4)$$

The first term is the kinetic term, and the second term is the gluon field self-interaction (also with strength g) is a unique feature of the non-Abelian gauge field.

Asymptotic freedom and confinement Due to quantum fluctuations, the effective coupling constant g changes with the energy scale of a process. The rate of change of g with respect to the scale parameter is called the β -function,

$$\frac{\partial g}{\partial \ln \mu} = \beta(g), \quad (1.5)$$

which can be evaluated as a perturbation series of g . At leading order, the QCD β function with number of colors N_c and n_f flavors of fermion is,

$$\beta(g) = - \left(\frac{11}{3} N_c - \frac{2}{3} n_f \right) \frac{g^3}{16\pi^2}. \quad (1.6)$$

This β function is negative for QCD ($N_c = 3$) using realistic numbers of quark flavors $n_f = 2 \cdots 6$, meaning the effective coupling constant decreases with increasing energy scale. The property is known as the asymptotic freedom of QCD because the interaction becomes small at asymptotically high energy, which also makes possible the use of perturbation theory at high energy.

Often a strong coupling constant is defined as $\alpha_s = g^2/4\pi$. Using the leading order β -function, its scale dependence is

$$\alpha_s(Q^2) = \frac{4\pi}{\left(\frac{11}{3}N_c - \frac{2}{3}n_f\right) \ln\left(\frac{Q^2}{\Lambda^2}\right)}. \quad (1.7)$$

The integration constant has been absorbed into the QCD scale parameter Λ . Therefore, at least in perturbation theory, Λ becomes the only parameter of QCD. Its value is determined by anchoring $\alpha_s(\mu)$ to the experimental measurement at a fixed scale, for example, $\alpha_s(M_z) = 0.1185$ at the scale equal to the Z boson mass. The leading order Λ is then around 200 MeV.

The decreasing of $\alpha_s(Q)$ is logarithmic slow at high energy, but it rises quickly approaching with Q approaching Λ from above. Even before reaching

this scale, the coupling constant is already too large for a reliable perturbative calculation. Near the Λ scale, QCD enters the non-perturbative region, and at this long distances only hadrons exists as colorless bound states of quarks and gluons. The fact that colors not directly observed at large distances is knowns as “color confinement” of QCD. To pull a quark out of the hadron, the color field becomes so strong that eventually more quark-anti-quark pairs populated in-between the pulled quark and the remnant and forms new colorless hadrons.

Depending on its valance quarks (quarks that carry the net quantum number of the hadron) content, hadrons are generally categorized as baryons and mesons. Baryon has three valance quarks or anti-quarks, such as neutrons and protons. Meson has a valance quark and an anti-quark, such as pion and kaon. Hadrons are also populated with sea-quarks and gluons that are constantly produced and annihilated as quantum fluctuations. The momentum of hadron is mostly carried by the valance quarks. The sea quarks and gluons together share the rest fraction of the total momentum, but their abundance number at high energy is very important for the particle production in relativistic hadron / heavy-ion collisions.

Nowadays, the only reliable ab initio theoretical tool for non-perturbative QCD is lattice field theory technique, where the QCD Lagrangian is discretized on a finite lattice and studied on a computer.

The phase-diagram of the QCD matter At zero temperature (T), protons and neutrons (together as nucleons) form bound states of atomic nuclei that build the ordinary matter. One can also define the baryon chemical potential μ_b , and for ordinary matter μ_b is around 1 GeV, close to the proton mass. The ordinary nuclei is indicated as the white dot on the (partly conjectured) phase diagram in figure 1.1 []. Increasing the temperature of the system, nucleons start escape from nuclear potential and other hadrons can be created from collision and resonance formation and decay. This system is know as the hadron gas (cyan region in figure 1.1).

Because QCD has asymptotic freedom at high energy and confinement at low energy scale, there can be so-called deconfinement phase-transition when temperatures crosses the QCD non-perturbative scale. At asymptotically high temperature, the weakening of the coupling should lead to the transit from the color confined hadronic matter to a system of transporting quarks and gluons, termed the quark-gluon plasma (QGP). Frist principle lattice QCD calculations have studied this transition at zero baryon chemical potential with 2+1 flavors (up / down plus strange quark) QCD. Figure 1.2 quotes the equation of state computed by the HotQCD Collaboration []. It

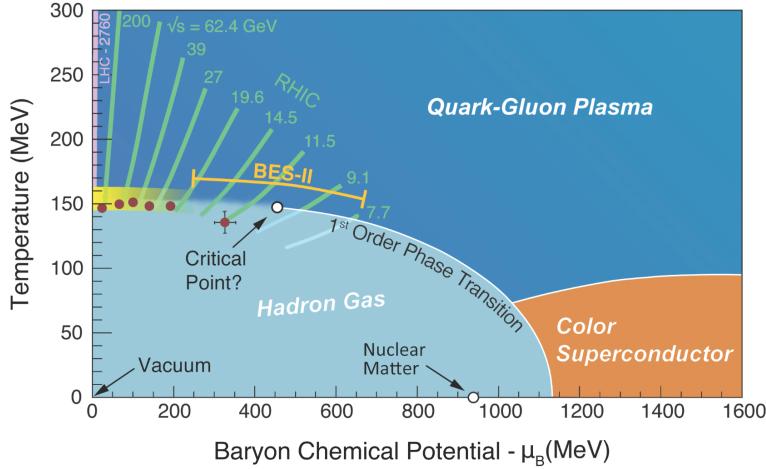


Figure 1.1 The (partly projected) phase-diagram of the nuclear matter from reference [1]. The horizontal variable is Baryon chemical potential μ_B and the vertical variable is temperature T . The red and green trajectories indicate the reachable regions by the heavy-ion program at the LHC and RHIC.

shows the pressure P , energy density (ϵ) and entropy density (s) of QCD system. These thermodynamic quantities are scaled by powers of temperature, so that the ratio can be loosely related the effective number of degrees of freedom (DoF) of the system. The Stefan-Boltzmann limit (non-interacting gas of quarks and gluons) is denoted as the dashed lines in the up-right corner. It is observed that the effective number of DoF converges to the expectation from a hadron resonance gas model (solid lines) at low temperature and rapidly increases to a value close to the Stefan-Boltzmann limit in a narrow temperature window. This suggests a releasing of the quark and gluon degrees of freedom at high temperature. More close study indicate that this is not a real phase-transition at $(\mu_b = 0)$, and sometimes people also refer to it as a “cross-over” phase transition, where the thermodynamical quantity is smooth across this region of phase-diagram. Nevertheless, a pseudo critical temperature is defined to be $T_c \approx 150$ MeV, corresponding to 1.5 trillion Kelvin.

Moving towards finite baryon chemical potential, the lattice approach runs into the fermion sign problem, though recent studies has been pushing the realm of lattice QCD into small μ/T regions [2]. Effective models [3] and Dyson-Schwinger equation studies [4] have suggested the existence of a first order phase transition at large μ_B/T . If true, the first-order coexistence line must end at a point on the phase-diagram at lower μ_b , beyond which the

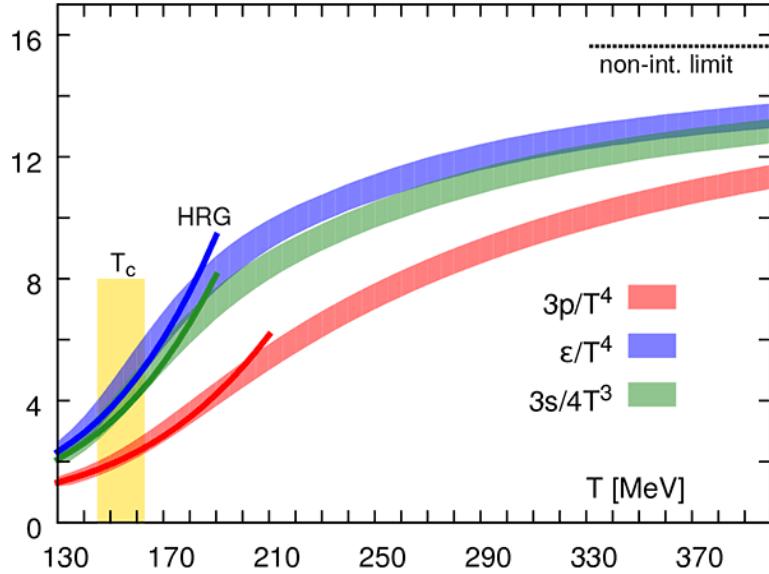


Figure 1.2 The lattice equation of state for 2+1 flavor QCD taken from reference [1]. The rescaled pressure, energy density and entropy density as function of temperature at zero chemical potential are shown as red, blue and green bands. The dashed lines indicates non-interaction (Stephan-Boltzmann) limit and the solid lines show the expected values from a hadron resonance gas. The yellow band is the region of pseudo-critical temperature.

phase-transition is the cross-over type. Such a point, called the critical end point (CEP), has attached a great interest of both theoretical confirmation / exclusion and experimental search.

At higher chemical potential and low temperature, another phase of nuclear matter known as the “color superconducting phase” is proposed, where the quarks forms Cooper pairs in analogy to the superconductors [2].

It is believed that the QCD high-temperature phase-transition is a stage of the universe around a microsecond after “the Big Bang”, when the temperature drops down to QCD scale. Compact starts are “celestial laboratories” to test the QCD equation-of-state in the high density and low temperature region, providing an important physical input for simulating the recently discovered gravitational wave from neutron star mergers. In laboratories, we create hot and dense nuclear matter by colliding heavy nuclei at ultra-relativistic high energies. Though the created matter is so transient and tiny compared to the cosmic nuclear matter, we can learn not only thermodynamic properties but also essential dynamical properties of the QCD in

these experiments.

1.2 Phenomenology of relativistic heavy-ion collision

Relativistic heavy-ion collision is currently the only tool to access high energy density QCD medium in laboratory. Since 2005, the Relativistic Heavy-ion Collider (RHIC) at the Brookhaven National Laboratory (BNL) started colliding gold nuclei at 200 GeV [1]. The Large Hadron Collider (LHC) started its heavy ion programs later, colliding lead nuclei at 2.76 TeV and 5.02 TeV [2]. Since then, many evidences have been pointing to the existence a new state-of-matter: the strongly coupled quark-gluon plasma (sQGP).

In this section, I shall introduce useful concepts and terminology in heavy-ion collisions. Then I will review a few important experimental evidences and how they can help the understanding of the properties of the sQGP.

1.2.1 Kinematics

In ultra relativistic collisions, it is advantages to use a new set of coordinates, related to the Cartesian coordinates by,

$$x_\perp = x_\perp \quad (1.8)$$

$$\tau = \sqrt{t^2 - z^2} \quad (1.9)$$

$$\eta_s = \frac{1}{2} \ln \frac{t+z}{t-z} \quad (1.10)$$

where the z direction aligns with the accelerated beam direction. τ is called the “proper time” and η_s called the space-time rapidity. One advantage of using this set of coordinates is that τ and η_s transforms much simpler than t and z under Lorentz boost (β_z) in the beam direction,

$$\tau' = \tau, \quad (1.11)$$

$$\eta'_s = \eta_s + \frac{1}{2} \ln \frac{1+\beta_z}{1-\beta_z} \quad (1.12)$$

Similarly for the four momentum p^μ is parametrized as

$$p_x = p_T \cos \phi \quad (1.13)$$

$$p_y = p_T \sin \phi \quad (1.14)$$

$$m_T = \sqrt{m^2 + p_T^2} \quad (1.15)$$

$$y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z}. \quad (1.16)$$

p_T is transverse momentum relative to the beam (z) direction, ϕ is the azimuth angle of particle emission. m_T is referred as the transverse mass, and y is the rapidity of a particle. Besides, pseudorapidity is often used in experiments,

$$\eta = \frac{1}{2} \ln \frac{|p| + p_z}{|p| - p_z} = \frac{1}{2} \ln \frac{1 + \cos \theta}{1 - \cos \theta} \quad (1.17)$$

It has the merits that it is directly related to the polar angle θ of particle emission. When the transverse mass is small compared to p_z , the pseudorapidity is also a good proxy of rapidity.

1.2.2 Nuclear collision geometry

Nuclei are extended objects. The radius of heavy nuclei approximately scales like $A^{1/3}$ fm, where A is the atomic number; therefore, the collision geometry plays far more important role than it is in the proton-proton collision. In the center-of-mass frame, nuclei “shrink” in the z direction by the factor $\gamma = (1 - v^2)^{-1/2} = E/M$ because of the Lorentz contraction. γ is over 100 for gold nuclei at top RHIC energy and is more than 2500 for lead nuclei at the LHC. As a result, the approaching nuclei takes a short time to penetrating each other $t_L = 2R/\gamma$, while dynamics in the transverse direction can only propagate within a causal circle of $r < t_L$ that is much smaller than the nuclear extend.

Impact-parameter and centrality Defining the impact parameter \vec{b} as the transverse separation between the center-of-mass of the two approach nuclei, the initial deposition of the energy largely depends on \vec{b} . The collision geometry is a useful handle to study QGP dynamics; however, it is impossible control b directly in high energy experiments. What is used as an approximate geometry indicator is the so-called centrality. Centrality are defined in different ways (detector response / multiplicity / transverse energy) and with different kinematic cuts, but the idea that nuclear collision geometry strongly correlates with the particle production activity. It is

reasonable to anticipate that the average number of charged particles produced or the total transverse energy deposited within a certain detector’s acceptance is higher if the collision is more central (small impact parameter), and is lower for peripheral collision (large impact parameter). Of course the relation between centrality and impact-parameter is not exact, as dynamical fluctuations smear out the one-to-one correspondence between the impact parameter and the “centrality meter”. Correctly accounting for these fluctuations is particularly important for small collision systems such as proton-lead and deuteron-gold collisions.

Centrality selection Experimentally, a minimum-biased (a minimum set of event triggers) sample of recorded events are sorted according to the centrality definition (multiplicity, e.g.) and the events are binned by percentile. Then, for example, the top 0–5% highest multiplicity events are associated to the central collisions with centrality range 0–5%. And the details of the collision geometry can be studied through a model. Usually, the models is one of the many variants of the Glauber model [], we shall explained it in detail in section ??). It computes the number of binary nucleon-nucleon (N_{bin}) collisions and number of participant nucleons (N_{part} , nucleons that suffers at least one binary collisions) at a given impact parameter. Experimentally, N_{part} is often used as the centrality estimator of the model as it is roughly proportional to the bulk particle production; while the cross-section of hard processes that involves large momentum transfer $Q \gg \Lambda$ scales like the N_{bin} . Though this correspondence can be model dependent, but the uncertainty can be quantified and its prediction can be validated by the production of colorless probes.

1.2.3 Particle production at low- p_T and collective flow

Immediately after the nuclei penetration through each other $t \sim 2R/\gamma$, huge amount of energy is deposited into the overlapped area and entropy is produced, creating a fireball in the middle while the nuclear remnants recede. This highly excited fireball of fields undergoes complex dynamics and cools down rapidly because of the longitudinal and transverse expansion. Eventually, the system hardronizes, and the hadrons can have further interactions and may decay into other hadrons, photons and lepton that are seen by the detectors.

It is observed that the particle production in relativistic nuclear collisions distributes across a wide (pseudo)rapidity range, and has steep falling transverse momentum spectra []. The majority of the particles are soft

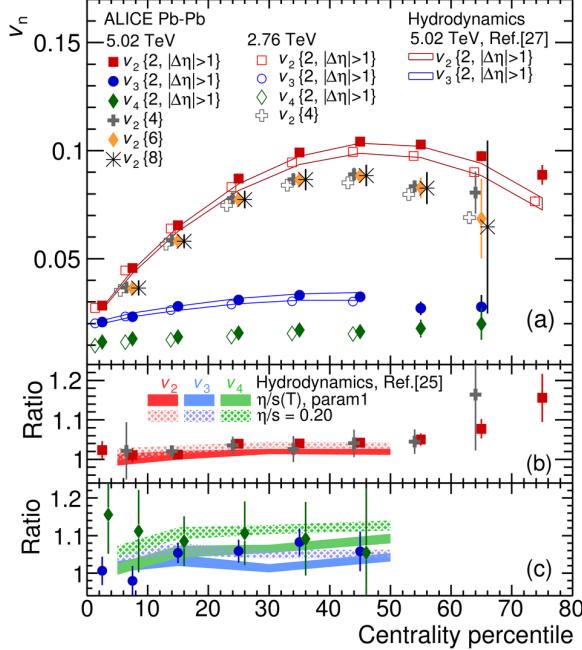


Figure 1.3 The momentum anisotropy coefficient v_2 estimated from multi-particle correlation for charged particle from the ALICE collaboration [1]. The hydrodynamic-based calculations [2] (lines) very well explains the centrality dependence of the second (red), third (blue) and fourth (green) order coefficients at different beam energies.

hadrons with relatively small transverse momentum $p_T \lesssim 3$ GeV and their creation are consequences of final state interactions [1]. One of the most striking discoveries from RHIC and LHC heavy-ion program is that these soft particles displays a strong collectivity and the patterns can be described by hydrodynamic-based models to a very high precision [1]. This success of the hydrodynamic model reveals the strongly coupled nature of the matter produced with a temperature several times above T_c and it has been entitled the name strongly coupled quark-gluon plasma. This is in contrary to a weakly coupled gas of quarks and gluons that emits independently.

One manifestation of collectivity is the momentum space anisotropy or collective flow of the bulk medium. Decompose the charged particle spectra into Fourier series of the azimuthal angle,

$$E \frac{dN}{p_T dp_T d\phi dy} = \frac{1}{2\pi} \frac{dN}{p_T dp_T dy} \left(1 + 2 \sum_{n=1}^{\infty} v_n(p_T) \cos[n(\phi - \Psi_n)] \right). \quad (1.18)$$

The first term is averaged yield, and subsequent terms in the sum encode the angular dependence. The $n = 1$ term is a shift of the center-of-mass momentum. From $n = 2$, v_{ns} are momentum anisotropy coefficients of $\cos(n\phi)$ modulations. If the particle production is simply an independent sum of elementary nucleon binary collisions, then the anisotropy would be zero after average. However, experiments observe a surprisingly larger elliptic flow (v_2), triangular flow (v_3) and higher order v_n at both RHIC and LHC in nuclear collisions. Figure 1.3 shows the variation of the v_n as function of centrality from ALICE measurements [1]. The v_2 coefficients first increases from central to mid-central collisions and slightly decreases at peripheral collisions, while v_3, v_4 signal are smaller and varies slower with centrality.

In the hydrodynamic picture, a non-central collision deposits initial energy density in an almond shape and the initial fireball has a finite spatial eccentricity ϵ_2 . The energy density is higher in the middle and lower at the boundary, so a hydrodynamic pressure builds up and drives the transverse expansion of the fireball. Because the pressure gradient is larger in the short axis-direction and the long-axis direction, the matter flows in an isotropic way, creating the observed momentum space second-order anisotropy v_2 . The existence of higher order of flow harmonics and non-zero v_2 in the most central collisions is because the nuclear configuration fluctuations, such as randomized nucleon positions, create all order of eccentricity ϵ_n . In short, a hydrodynamic expansion transfer initial geometry eccentricities ϵ_n into final state momentum anisotropy v_n of the particle.

Extracting the QGP transport coefficients A relativistic ideal hydrodynamic model assumes an infinitely strong interaction that the medium always stages in local thermal equilibrium. A more sophisticated treatment is the relativistic viscous hydrodynamics to account for deviations from the local thermal equilibrium due to large gradients in the expansion. The response of hydrodynamic evolution to the gradients are characterized by the shear viscosity η and bulk viscosity ζ . The QGP shear viscosity and bulk viscosity are of fundamental importance. The shear viscosity to entropy ratio η/s is an indicator of the stong / weak coupling nature of the QGP. And the bulk viscosity to entropy ratio ζ/s is directly related to the scale-invariance breaking of QCD.

Dynamical quantities such as viscosity are extremely hard to be computed from first principle, so currently, the pinning down of these numbers and their temperature dependence resorts to the phenomenological extraction from experiments [1–6]. The flow harmonics v_n are particular sensitive to the viscous effects, as a finite viscosity damps the development of

anisotropic flows, reducing the transition efficiency from ϵ_n to v_n . Global comparisons of the state-of-the-art medium modeling to a collection of soft observables have corroborated the need of a small η/s that are likely to be slowly increasing with temperature and a non-vanishing ζ/s .

1.2.4 Probing sQGP using hard probes

Very occasionally, an initial collision involves large momentum transfer creates high- p_T particles in the system ($p_T \gtrsim 10$ GeV), are referred to as the “hard” particles. By uncertainty principal, they can only be produced at the beginning of the nuclear collision on a time scale $\delta t \sim 1/p_T$, then they pass through and interact with the surrounding bulk medium. Hard particles can be used as self-generated probes of the system. Due the asymptotic freedom, the initial production of hard processes can be computed in the perturbative framework, granting a good theoretical control of its initial state. The final state interaction with the medium then modifies the initial production and leaves finger prints of the medium on the hard probes.

Jet and jet quenching Initial hard partons (gluons, quarks) undergoes complex QCD dynamics, radiating more partons which then hadronizes into a collimated bunch of hadrons and decay products. This final collection of particles is observed in detector as jets. In the proton-proton collisions, perturbative calculations and Monte-Carlo simulations are able to explains the production cross-section of the jet and leading hadrons (the hardest hadron in the jet) reasonably well. In the nuclear collisions, the initial parton and the radiative daughter partons interacts with the medium, causing energy loss and triggering medium-induced radiation. As a result, one expects the jet / leading parton yield at high- p_T is reduced compared to the reference in proton-proton. To focus on the difference caused by medium effects, the reference has to cancel out a naïve difference that simply rises because there are more effective nucleon-nucleon collisions than the proton-proton collisions. One defines the so-called “nuclear modification factor”,

$$R_{AA}(y, p_T) = \frac{\frac{dN_{AA}}{dydp_T}}{\langle N_{\text{coll}} \rangle \frac{dN_{pp}}{dydp_T}} = \frac{\frac{dN_{AA}}{dydp_T}}{\langle T_{AA} \rangle \frac{d\sigma_{pp}}{dydp_T}}. \quad (1.19)$$

It is the average N_{bin} “normalized” ratio between the yield in AA collisions and pp collision. The number of binary collision is sometimes replaced by the average nuclear overlapping function $\langle N_{\text{coll}} \rangle = \langle T_{AA} \rangle / \sigma_{pp}^{\text{inel}}$, and the yield is replaced by the inclusive cross-section for the proton-proton collision $\frac{dN_{pp}}{dydp_T} \rightarrow \frac{d\sigma_{pp}}{dydp_T}$. These two expressions are equivalent. The ratio is expected

to be unity if there is no medium effect, though we do remind the readers that N_{coll} is not a directly observed quantity and has to be estimated in a model-dependent way.

At both RHIC and the LHC, colored probes as measured by the R_{AA} of leading hadron and jet are found to be significantly below unity in nuclear collisions, while R_{AA} of color neutral probe such as Z -boson is consistent with unity. These discoveries indicate the creation of a color deconfined medium that strongly modifies to hard parton propagation. The interaction strength between the hard parton and the medium is theoretically quantified as the jet transport parameter \hat{q} , which is defined as the momentum broadening per unit path-length in the transverse direction of the propagation,

$$\frac{d\langle p_\perp^2 \rangle}{dL} = \hat{q} \quad (1.20)$$

The jet transport coefficients is another quantity of fundamental interest in heavy-ion collisions, and there has been a great effort in both first principal computation and phenomenological extraction. The hard parton / jet probes the medium at different scale at different stage of its evolution, and more sophisticated observables and theoretical tools are being constructed to answer more microscopic questions such as the actually degrees of freedom of the strongly coupled QGP [].

Heavy-flavor probes Heavy flavor is a charming probe in studying heavy-ion collisions, and is also the focus of this work. Heavy quarks have mass well above the QCD non-perturbative scale. The charm quark ($M = 1.3$ GeV) and bottom quark ($M=4.2$ GeV) are the most relevant heavy quarks for the present study. The reason that top quark ($M = 173$ GeV) is out of our discussion is due to its extremely short life time ($\sim 5 \times 10^{-25} \approx 0.15$ fm/ c in its rest frame) so it barely interacts with the QGP before it decays into, predominantly, bottom quarks. Though there has also been proposal that takes the advantage of this short life-time to probe the temporal structure of the QGP evolution, we only focus on the charm and bottom flavor in this work.

A large mass guarantees a negligible thermal production contribution, at least for the present top LHC beam energies (there are estimations that thermal contribution can play a role in future FCC collider []). Therefore, heavy flavors, regardless of its p_T , are almost always created in initial hard processes. Moreover, the tiny population of heavy flavors in the collision also suppresses the chances that they annihilates / recombine with their anti-particles. Certainty heavy mesons have a long life time such that the

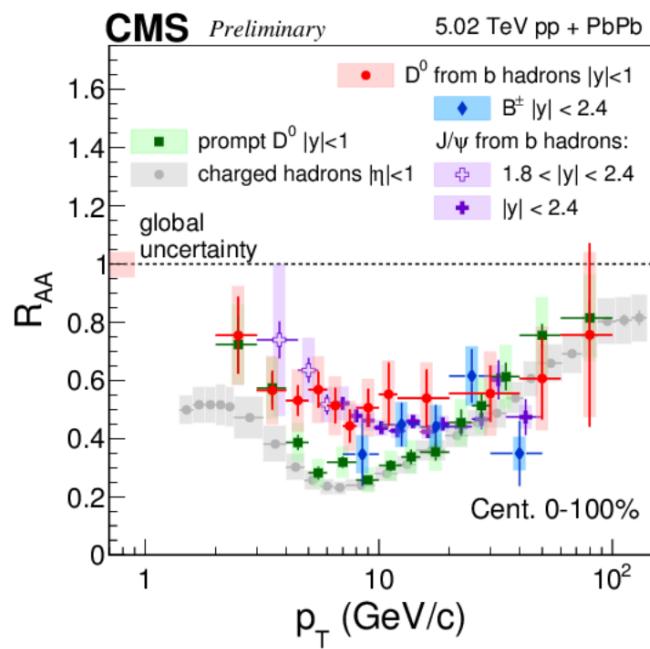


Figure 1.4 The nuclear modification factor $R_{AA}(p_T)$ of charged hadron (gray), D meson (red), B meson (blue), and b -decayed D meson (red), b -decayed J/Ψ (purple) measured by the CMS collaboration [1].

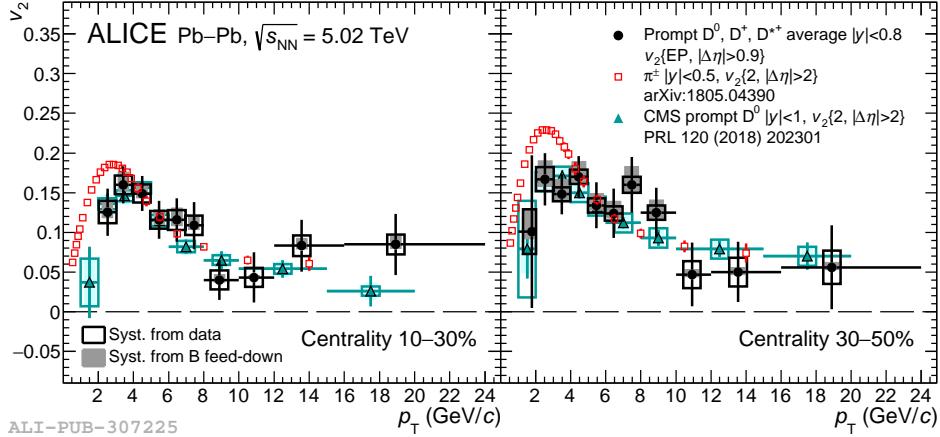


Figure 1.5 The charged pion (red) and D meson momentum anisotropy measured by the ALICE Collaboration (black) and the CMS Collaboration (green). Left and right panels show the results for 10-30% centrality and 30-50% centrality respectively.

decay vertices are outside of the fireball and can be resolved by experiments. Therefore, the number of heavy-flavor particles is almost conserved from the beginning to the end of the entire medium evolution including both the QGP phase and the hadronic phase.

Heavy flavors are of physical interests in many ways. The mass effects are negligible at high p_T where heavy flavors merge into the topic of the jet energy loss physics. At intermediate p_T , the mass effect is expected to suppress the medium-induce radiation, which dominates the energy loss of light quark. And there may be a competing between the collisional energy loss and radiation processes. Experimentally, these differences lead to a hierarchy in the amount of nuclear suppression. For example, figure 1.4 citing from the CMS collaboration shows a collection of R_{AA} measurements, for charged (mostly light) hadron, prompt D meson, prompt B meson and D and J/Ψ from b -decays. All the R_{AA} tends to collapse onto the same trend at very high- p_T , while for p_T range around 5 to 20 GeV, despite the large uncertainty, there is a suggestive hierarchy of $R_{AA}(\text{light}) < R_{AA}(\text{charm}) < R_{AA}(\text{bottom})$. It would be interesting to study whether the theoretical framework can explain this difference quantitatively and distinguish different energy loss mechanisms.

Low- p_T heavy quark physics is even more interesting. In this region, collisional process dominates over radiative process, and the description of

the heavy quark dynamics under the influence of medium “kicks” reduces to the succinct diffusion equation [1]. A spatial diffusion constant D_s controls the close-to-equilibrium dynamics, and can be related to the momentum diffusion by $D_s = 4T^2/\hat{q}(p \rightarrow 0)$ [1]. The large inertia $M \gg T$ delays its relaxation time $\tau_{\text{th}} \propto M/TD_s$ and one expects to find a different degree of thermalization for light, charmed, and bottom hadrons. For instance, looking at the low p_T momentum anisotropy of charmed meson shown in figure 1.5 [1]. The large v_2 of the charged pions below 3 GeV is due to the collective expansion. The charmed mesons also catch up a significant amount of flow ¹, though still less than the pion. To explain this amount of D meson v_2 , phenomenological studies suggest a D_s close to the lattice QCD evaluations [1], while leading order weakly coupled results [1] is inadequate. This finding suggests the importance of non-perturbative phenomenon in understanding the coupling between low momentum heavy quark and the medium [1].

Finally, the unique flavors of heavy quarks help to tag certain processes of interest. For example, the study of recombination hadronization mechanism, strange ness enhancement, and implementing a selection bias on the quark / gluon-initiated jet ratio [1].

1.2.5 Transport modeling of hard probes

The understanding of jets and heavy-flavor in heavy-ion collisions needs a comprehensive non-equilibrium modeling. This includes initial production / DGLAP evolution, the partonic propagation in the QGP, and eventually the hadronic interaction. Transport equations are convenient tools to couple the microscopic hard probes propagation to the macroscopic medium evolution, though one have to be very careful with the multiple scales of the problem. For example DGLAP evolution brings the parton scale from p_T down to $O(\text{GeV})$. The probe-medium interactions happens at typical scales around temperature T and the screening mass $m_D \sim gT$, while the medium-induced radiation suffers momentum broadening scale of order $\hat{q}t$. Eventually, hadronization happens at scale Λ . Meanwhile, the medium evolution has another set of (time) scales, the hydrodynamization time $\sim 1 \text{ fm}/c$, the finite-size and life-time of the QGP fireball $\sim O(10) \text{ fm}/c$, and the expansion time scale τ_{ex} . Usually a well separation of scales allows great simplification to the theory calculations. For example, the Boltzmann transport equation requires a separation between the mean-free-path and the coherence time of the scattering. However, in realistic event simulations, treating

¹As a remark, the finite v_2 of D meson at high p_T is not directly related to the flow phenomena, but as a result of anisotropic energy loss in a spatial eccentric medium

regions of overlapping scales seems inevitable. We would like to develop in this thesis a new transport model to account for a few of these overlapping scale issues.

Heavy quark transport models In early days, the heavy quark measurements at RHIC energy does not extend to very high- p_T and the radiative energy loss is not as important as elastic ones. And one study the non-equilibrium dynamics using a pure diffusion model [1]. To include physics at high- p_T physics, a radiation improved diffusion model was then developed [2] and has been applied to the first Bayesian extraction of the heavy quark transport coefficients [3]. Apart from the diffusion-based models, Boltzmann and linearized Boltzmann models, including both elastic and inelastic interactions, are also developed [4]. Regarding the physical inputs, the Boltzmann-based model takes a weakly-coupled picture; the diffusion based model is more flexible, since the transport coefficient can be computed in both weakly coupled or strongly coupled approach [5]. Using different models, the extracted transport parameters D_s , \hat{q} have notable differences [6]. The major sources that leads to these differences are:

- Whether the radiative energy loss is included.
- Assumptions on the medium: close-to-equilibrium hydrodynamic medium, or non-equilibrium form full partonic Boltzmann equation.
- Weakly coupled approach versus strongly coupled approach.
- More subtle differences such as Langevin versus Boltzmann dynamics, and the detailed treatment of the radiative process.

To make convergent progress, on the one hand improved theoretical calculations and more accurate modeling is important; on the other hand, more subtle differences should can be treated as intrinsic modeling uncertainty so that the extracted transport parameters are not over-interpreted (a finite theoretical uncertainty bands on D_s and \hat{q}). I will also try to make progress in this direction.

1.2.6 Understanding QGP as a parameter inference problem

All the interesting dynamics of heavy-ion collision only last for $O(10)$ fm/ c , while we can only observe the collision remnants by detectors meters away. Therefore, the learning of any intrinsic properties of QGP is essentially a parameter inference problem: given measurements, models, and parameters

of QGP such as η/s , \hat{q} , what is the favored range of parameters to explain the data. Finally, by comparing the theoretical expectations (if exists) and the phenomenological constraints of these parameters, one evaluate the theoretical assumptions, which gives out new information of the QGP.

This inversion from observables to parameters is not as simple as it appears, because of the following difficulties,

- The dynamical models are complex and computationally intense.
- Model takes multiple parameters or unknown functions that have infinitely many degrees of freedom.
- Global comparison to many experimental observables.
- The quantification of uncertainty: including experimental uncertainty, model uncertainty and theoretical uncertainty.

Most of these issues can be solved by the Bayes analysis for model parameter calibration, and its key ingredients will be explained in chapter 5. A remaining issue is the theoretical uncertainties, which is hard to quantify. Our solution to the theoretical uncertainty is two-folded. First, if there are more than one theoretical assumptions without appealing reasons to disfavor either of them, then this difference should be propagated into the extracted model parameters. Including these uncertainty will certainly decrease the constraining power on the transport parameters, but it prevents biasing the estimated number from imposing a too strong assumption. Second, existing theoretical calculations are often worked out in certain idealized limits, while a dynamical modeling is much more complicated and may not closely follow what the underlying theory. This will certainly obscure the interpretation of the extracted parameters. Therefore, as an important practice for dynamical modeling, the model should be able to calibrate to theoretical calculations at least in those idealized limits, and then generalized to the more complex scenario. We devoted chapter ?? to improve the accuracy of hard parton transport model.

1.3 Outline of this Thesis

In this thesis, I focuses on the extraction of the heavy quark transport coefficients from experiments using a newly developed transport model for hard parton in a quark-gluon plasma. In chapter 2, I introduce a hydrodynamic-based medium for the medium evolution. As an application of this sim-

ulation framework, I review my project on reverse engineering a three-dimensional initial entropy deposition of the heavy-ion collision from experimental data. In chapter 3, we develop the transport model for hard partons (including heavy flavors) propagation inside a quark-gluon plasma. This model interpolates a small-angle diffusion picture and a large-angle scattering picture of the probe-medium interaction. I show the limitation of the semi-classical transport approach in implementing parton branching processes (radiation) at high energy, and demonstrate how to modified the semi-classical approach to treat it properly. Chapter 4 builds a comprehensive simulation workflow that couples the initial production and in-medium transport of heavy flavors to the bulk medium evolution. Benchmark calculations with simple guesses of parameters are compared to the experimental measurements. Chapter 5 is a brief description of the Bayes methodology of model parameter calibration. Applying the Bayes method, in chapter 6, a systematic model-to-data comparison is performed, extracting the heavy flavor transport properties. Finally, chapter 7 summarizes the work and discuss possible future improvements.

2

Bulk medium evolution and initial condition

This chapter introduces a hydrodynamic-based model for the medium evolution in the heavy-ion collision. I will also review my project on applying this framework to reverse engineering the initial three-dimensional entropy deposition from experimental observables [7].

2.1 A Hydrodynamics-based dynamical modeling

2.1.1 Relativistic hydrodynamic

The relativistic hydrodynamics plays a center role in such a modeling. It is relativistic as the flow velocity of the QGP fire ball expansion can reach a significant fraction of the speed of light. It is a macroscopic description that propagates the energy momentum tensor of the system without a detailed knowledge of the microscopic interaction. The first set of equations comes from the the energy-momentum conservation, which should always be satisfied,

$$\partial_\mu T^{\mu\nu} = 0. \quad (2.1)$$

$T^{\mu\nu}$ is the energy momentum tensor and $\partial_\mu = \partial/\partial x^\mu$. Here we have choose the metric as $g^{\mu\nu} = \text{diag}\{1, -1, -1, -1\}$.

Ideal hydrodynamics Ideal hydrodynamics assumes that the system relaxes to local thermal equilibrium much faster compared to other time scale, then, $T^{\mu\nu}$ can be specified by given only the energy density e , pressure P ,

and flow velocity u^μ of a fluid element,

$$\partial_\mu T^{\mu\nu} = eu^\mu\nu - P(g^{\mu\nu} - u^\mu u^\nu). \quad (2.2)$$

Boosting into the co-moving frame if the fluid element, $T^{\mu\nu}$ reduces to the diagonal form $T^{\mu\nu} = \text{diag}\{e, -P, -P, -P\}$.

There are five unknowns e, P, u_x, u_y, u_z (u_t is determined by $u^2 = 1$), but conservation laws 2.1 only provide four equations. A fifth equation is the equation of state (EoS) $P = P(e)$, relating pressure and energy density in the thermal equilibrium, then the ideal-hydrodynamic equations are complete. Lattice QCD calculations has determined the 2+1 flavor QCD equation of state to a high precision. Though it is not a prior that the lattice QCD EoS computed in an infinite matter in an infinite time is the right choice for describing a transient system with a large gradients, using the lattice input does result in reasonable agreement with the data. Moreover, there has been a study that try to constrain the from of EoS from experimental data and the “calibrated” EoS is very close the Lattice calculation [8].

Viscosity hydrodynamics and QCD transport coefficients A physical relaxation rate is always finite, and the system can be driven out of local thermal equilibrium by the large gradients of the fast expanding fireball. Relativistic viscosity hydrodynamics taken into account the off-equilibrium effect by include viscous corrections. The energy momentum tensor deviates from the ideal one by a bulk viscous pressure Π , and a shear viscous tensor $\pi^{\mu\nu}$.

$$T^{\mu\nu} = u^\mu u^\nu e - (g^{\mu\nu} - u^\mu u^\nu)(P + \Pi) + \pi^{\mu\nu}. \quad (2.3)$$

The Π and $\pi^{\mu\nu}$ will then response to the finite gradients of the fluid field. To first order in the gradient, they are given by the constitutive relations,

$$\pi^{\mu\nu} = 2\eta\sigma^{\mu\nu}, \quad (2.4)$$

$$\Pi = -\zeta\theta, \quad (2.5)$$

and the hydrodynamic equation is the relativistic version of the Naiver-Stokes equations. Here, $\sigma^{\mu\nu} = \partial^{(\mu}u^{\nu)}$, $\theta = \partial \cdot u$ are the fluid shear stress and expansion rate. The proportional constant are known as the QCD shear (η) and bulk (ζ) viscosity, encoding dynamical information of the QCD medium. Their dimensionless ratio to the entropy density η/s and ζ/s are important indicator of the interaction strength and the scale-violation of the QCD matter and are of great physical importance. There have been many

effort to either computing these quantities from first principles and effective models or extracting these numbers from experiments [9–13].

Coming back to the hydrodynamic equation, it is shown that one has to go to second order in the gradient expansion to the render the viscous correction compatible with special relativity. Meanwhile, π , Π becomes dynamical quantities that relax to the Naiver-Stokes limit.

$$\begin{aligned}\tau_\pi \dot{\pi}^{\langle\mu\nu\rangle} + \pi^{\mu\nu} &= 2\eta\sigma^{\mu\nu} - \delta_{\pi\pi}\pi^{\mu\nu}\theta + \phi_7\pi_\alpha^{\langle\mu}\pi^{\nu\rangle\alpha} \\ &\quad - \tau_{\pi\pi}\pi_\alpha^{\langle\mu}\sigma^{\nu\rangle\alpha} + \lambda_{\pi\Pi}\Pi\sigma^{\mu\nu},\end{aligned}\tag{2.6}$$

$$\tau_\Pi \dot{\Pi} + \Pi = -\zeta\theta - \delta_{\Pi\Pi}\Pi\theta + \lambda_{\Pi\pi}\pi^{\mu\nu}\sigma_{\mu\nu}.\tag{2.7}$$

The $\tau_\pi, \tau_\Pi, \delta, \phi, \lambda$ are known as second order transport coefficients. This complicated set of equations together with the conservation law and the EoS forms the viscosity hydrodynamic equations. Nowadays, well tested numerical packages have been developed solving these equations in the context of heavy-ion collisions [5, 14–16].

Boost-invariance approximation and beyond In general, the hydrodynamic equations have to be solved as in 3+1 dimensions. But a reduction to a 2+1 dimension is possible, if a boost-invariant symmetry is assumed near mid-rapidity [17–22]. This symmetry is first proposed by Bjorken in [23] that the system at different space-time rapidity behaves the same upto a longitudinal boost, and is termed “boost-invariance”. Then, the 2+1 dimension solution obtained at one space-time rapidity ($\eta_s = 0$) can be boosted to get the solution at other η_s . As a result, particle emissions from such a fireball does not strongly depends on the η_s .

The η_s -dependence cannot be detected, but is related to the emitted particle rapidity / pseudo-rapidity for the reason below. Suppose that the Lorentz contracted nuclei interact at $z = 0$ and produce excitations that free-stream in the longitudinal direction, then for each of these excitation

$$\frac{z}{t} = \frac{p_z}{E}.\tag{2.8}$$

This approximation the equivalence of η_s and y at early stages of the collision:

$$\eta_s = \frac{1}{2} \log \frac{t+z}{t-z} \sim y = \frac{1}{2} \log \frac{E+p_z}{E-p_z}.\tag{2.9}$$

Assume further these initial excitations has a small mass, then the rapidity can be approximated by pseudorapidity as $E \approx |p|$. Since the following hydrodynamics is boost-invariant, then emitted particle pseudo-rapidity should be flat. Experimentally, the event-averaged rapidity-distribution of charged

particles dN_{ch}/dy in both proton-proton and symmetric nuclei-nuclei collisions at the RHIC and energy falls at large rapidity but has a central plateau at least within $|y| < 2$.

However, since dN_{ch}/dy are event-averaged quantities, its being flat within $|y| < 2$ does not rule out the event-by-event particle production fluctuation which breaks the boost-invariance, and these fluctuations can be different at different transverse locations. Moreover, asymmetric nuclear collision such as $p+Pb, p+Au, d+Au, He+Au$, etc clearly breaks the boost-invariance even on an event averaged level [24–34] Therefore, the study of longitudinal fluctuation related observables or the search for hydrodynamic behavior in small collision system clearly requires one to go beyond the boost-invariance set-up.

2.1.2 Particularization and microscopic transport

The longitudinal and transverse expansion cools down the system temperature. Density and relaxation rate also drops rapidly. Eventually the relaxation time is so long for the hydrodynamic approach to apply. At this point, it is more proper to switch to a microscopic transport model. This switching is usually done near or below the pseudo-critical temperature $T_{sw} \lesssim T_c$ so that the energy momentum tensor can be particularized as an ensemble of hadrons, whose interactions are well known. If this matching is performed well above T_c , then we will have to deal with the problem of modeling quark / gluon dynamics and hadronization in the strong coupled regime near T_c . Of course, whether a hydrodynamics with lattice EoS and a hadronic transport model with cross-sections as inputs are both valid in the $T_{sw} \lesssim T_c$ region is another question.

The hydrodynamic $T^{\mu\nu}$ is usually particlized at a constant energy density / temperature hypersurface using the Cooper-Frye prescription. The number of specie “a” particles emitted with momentum p from a hypersurface element i is computed from,

$$\Delta N_i^a(p) = \frac{g^a f^a(p) dp^3}{(2\pi)^3} \frac{p^\mu}{E} \Delta\sigma_{i,\mu}. \quad (2.10)$$

$f^a(p)$ is the phase space density, $\Delta\sigma_{i,\mu}$ is the four components of the surface element, which has a unit of a 3D volume, and g^a is degeneracy of the specie. This distribution function should include both a thermal part and a viscous correction, $f = f_0 + \delta f$. There are more than one way to construct the viscous correction δf from e, P, n, Π and $\pi^{\mu\nu}$ based on different assumptions of the non-equilibrium corrections. In this work, we use a non-additive δf

correction that has been developed in [35, 36] and implemented by [12]. Please refer to these references for the original formulation and numerical implementation details.

The particlized hadronic system is then solved by the Ultra-relativistic Quantum Molecular Dynamics (UrQMD) model [37, 38] until the system is dilute enough and interaction ceases (kinetic freezeout). The UrQMD model includes processes such resonance decays, elastic and inelastic scatterings, and string formations and fragmentations.

2.1.3 Pre-equilibrium stage

At very early times of the collision, the system is off equilibrium. However, viscous hydrodynamic assumes a closeness to the local thermal equilibrium . (There are also recent efforts in understanding the effectiveness of hydrodynamics outside of its traditional range of application [39–41]). A successful prediction using an early onset of hydrodynamic evolution at $\tau_0 \lesssim 1\text{fm}/c$ suggests a fast hydrodynamization, though the mechanism is still a debatable. There are different modelings of the pre-equilibrium stage¹, including solving the classical Yang-Mills equation [19, 42], applying partonic transport models [43], a collision-less Boltzmann equation (free-streaming) plus Landau matching [44], and the linear response method of the effective kinetic approach [45].

Here we briefly introduce the free-streaming model [44]. The initial energy density ($\tau = 0^+$) at mid-rapidity is thought to be carried by massless partons that propagates at the speed of light in the transverse direction. The initial distribution function is put into factorized form $f(x_\perp, p_\perp, \tau = 0) = n(x, \tau = 0) \times dN/dp_\perp^2$. The momentum distribution dN/dp_\perp^2 does not evolve with time as the collisions are neglected, while the spatial density propagates as

$$n(\vec{x}, \tau) = \int n(\vec{x}', \tau = 0) \delta^{(2)}(\vec{x} - \vec{x}' - \tau) d\vec{x}'^2 \quad (2.11)$$

Then, the model assumes a sudden hydrodynamization at time τ_{hydro} , where the free-streamed,

$$T^{\mu\nu}(x_\perp, \tau_{\text{hydro}}) = \int f(x_\perp, p_\perp, \tau = 0) \frac{p^\mu p^\nu}{E} dp^3 \quad (2.12)$$

¹Such a pre-equilibrium stage was not included in my study of the 3D initial condition, and the hydrodynamics starts at $\tau_0 = 0.6 \text{ fm}/c$ assuming local thermal equilibrium. For my later study of the heavy flavor transport, a 2+1D collision-less Boltzmann equation implemented by [12] is used.

is used for initializing the hydrodynamic equations by the Landau matching procedure [44].

2.2 Initial condition model

Unlike the dynamical models that are governed by a few equations / laws with a few parameters, the initial condition model parameterizes many more unknowns. For different initial condition models, these unknowns can be initial color density of the nuclear wave function, the effective size of a nucleon, the form factor of nucleon-nucleon inelastic cross-section, and the amount of fluctuations in particle production / energy deposition, etc. There are two classes of initial condition models:

- Models that takes into the particle production dynamics. Such as minijet production, strings productions and flux-tubes, coarse-grained hadronic transport model, and color-glass condensate (CGC) effective field theory based models.
- Parametric models. Models provide macroscopic initial conditions without a dynamical component. Such as Monte-Carlo Glauber models and its extensions, and the T_RENTo initial condition model to be explained.

This section introduces the original boost-invariant T_RENTo model, and my work that extends the model to include longitudinal fluctuations.

2.2.1 The original (boost-invariant) T_RENTo model

The original T_RENTo model is proposed as a flexible ansatz to investigate a family of entropy / energy deposition behaviors at mid-rapidity.

First, the impact parameter \vec{b}_{AB} between the two colliding nuclei A and B is sampled at random. Then, the nucleons positions inside each nuclei are sampled according to the Woods-Saxon distribution ²,

$$\frac{df_N}{r^2 dr d\phi d \cos \theta} = \frac{1}{\exp\left\{\frac{r - R(1 + \beta_2 Y_{20}(\theta) + \beta_4 Y_{40}(\theta))}{a}\right\} + 1} \quad (2.13)$$

²The Woods-Saxon distribution is intended for heavy nuclei, for light nuclei such as Deuteron, Helium, Oxygen, the two-wave function or pre-tabulated nuclear configuration is used for sampling

including the quadrupole and hexadecapole deformation of certain nuclei. The randomized nucleon position is critical to explain the odd order of flow harmonics observed in experiments [46].

The collision between the two nuclei is determined at the nucleon level. Every nucleon pair $\{i, j\}$ with i from nuclei A and j from nuclei B has a certainty probability to collide inelastically. This probability at given nucleon-nucleon impact parameter $\vec{b}_{ij} = \vec{b}_{AB} + \vec{x}_{i,\perp} - \vec{x}_{j,\perp}$ is parametrized as,

$$P(b_{ij}; \sigma) = 1 - \exp [-\sigma T_{pp}(b_{ij})], \quad (2.14)$$

where $T_{pp}(b)$ is the overlapping function between the z -integrated density of the nucleon T_p ,

$$T_{pp}(b) = \int d\vec{x}_\perp^2 T_p(\vec{x}_\perp - \vec{b}/2) T_p(\vec{x}_\perp + \vec{b}/2). \quad (2.15)$$

Assuming a 3D Gaussian shaped nucleon with width parameter w , T_p is,

$$T_p(\vec{x}_\perp^2) = \frac{1}{2\pi w^2} \exp \left(-\frac{\vec{x}^2}{2w^2} \right). \quad (2.16)$$

w is treated as a tunable parameter. The σ parameter in equation 2.14 is the nucleon opacity parameter with units of an area. It is determined by fitting to the experimental measured proton-proton inelastic cross-section at a given beam energy,

$$\sigma_{pp}^{\text{inel}}(\sqrt{s}) = \int d\vec{b}^2 P(b; \sigma(\sqrt{s})). \quad (2.17)$$

Apply the probabilistic collision criteria of equation 2.14 to each pair of nucleons and sample the binary collisions. Nucleons that suffer at least one inelastic collisions are called participants and the total number of binary inelastic collisions are denoted as N_{bin} . The minimum-biased event sample in the TRENTo model are defined as all events that has at least one binary collision.

The above procedure is similar to the that of an Monte-Carlo Glauber model in determine the nuclear inelastic cross-section. Some experimental version of the Glauber model uses a black disk proton instead of a Gaussian profile. We found that this differences results in little change in the centrality dependence of N_{part} , but can greatly affects N_{bin} and may affects the computation of hard probe nuclear modification factor.

The novel component of TRENTo is an ansatz that maps from the participants to the energy / entropy density deposited at the mid-rapidity. Define the participant densities as a sum of the participants' thickness function,

$$T_{A,B}(\mathbf{x}) = \sum_{i \in \text{Parts}_{A,B}} w_i T_p(\mathbf{x} - \mathbf{x}_i). \quad (2.18)$$

The summation goes over the all participants in nuclei A and B , and each contribution is modulated by a fluctuating weight w_i that follows a Γ -distribution. The fluctuation has with unit mean and variance $1/k$ and k is a free parameter. This weight accounts for the large multiplicity fluctuation in the minimum biased proton-proton collisions. The entropy / energy density deposit at mid-rapidity is assumed to be a function of T_A and T_B only at each transverse location,

$$\frac{dS(\vec{x})}{d\eta dx_\perp^2} \text{ or } \frac{dE(\vec{x})}{d\eta dx_\perp^2} = f(T_A(\vec{x}), T_B(\vec{x})). \quad (2.19)$$

This simplification is possible because at $\tau = 0^+$, causality requires that the entropy production at one location cannot be correlated with the information at a different transverse location. Also, the partons that contribute to the bulk low- p_T particle production at high \sqrt{s} are predominately low energy gluons whose longitudinal wavelength is longer than the contracted proton radius in the z -direction; therefore, the entropy production should not be sensitive to the details of how the participants aligned but only its z -integrated density. TRENTo parametrizes this mapping from T_A and T_B to the energy / entropy deposition using a “generally mean” ansatz,

$$f(T_A, T_B; p) = \left(\frac{T_A^p + T_B^p}{2} \right)^{1/p}. \quad (2.20)$$

p is another tunable parameter. Some special values of p reduces the ansatz to the well known average procedures as shown in table 2.1. This way the model is able to parametrize a class of entropy / energy production scheme and includes certain type of initial condition uncertainty. Through a global model-to-data comparison, this p parameter has been calibrated to be very close to 0, suggesting the data favors a mid-rapidity entropy / energy deposition that scales as $(T_A T_B)^{0.5}$. A similar scaling is also found in the EKRT initial condition model based on pQCD particle production and saturation physics [47].

Table 2.1 T_RENTo p -parameter

$p \in \mathbb{R}$	$f(x, y)$	Entropy / energy production
$-\infty$	$\min\{x, y\}$	dominated by the thinner target
-1	$2xy/(x + y)$	the harmonic mean scaling
0	\sqrt{xy}	the geometric mean scaling
1	$(x + y)/2$	the arithmetic mean (participant) scaling
$+\infty$	$\max\{x, y\}$	dominated by the thicker target

2.2.2 Parametrize the longitudinal dependence in T_RENTo

The T_RENTo model has been doing successful phenomenology for obserables at mid-rapidity [10, 21, 48]. My work focuses on extending the parametrization to a rapidity-dependent initial condition, and seek for a reverse-engineered 3D entropy production from the rapidity-dependent observables [7].

A strong source that breaks the boost-invariance is the initial asymmetric participant density $T_A \neq T_B$; in addition, dynamical fluctuations can generate asymmetry as well. We listed what contributions are included and what are not in the model

- In asymmetric collisions like p - A and non-central A - A , the local thickness functions are imbalanced $T_A \neq T_B$.
- Even in central A - A collision, nuclear / nucleon configuration fluctuation also contributes to the asymmetry. It is included as the randomized nucleon position fluctuation and the γ -fluctuation of the nucleon thickness function.
- Initial stage dynamical fluctuation, initial flow in the z -direction are not included.

Therefore, the asymmetry in the extended T_RENTo model only comes from the imbalanced T_A and T_B . Take the following decomposition of $s(\mathbf{x}, \eta_s)$ at the hydrodynamic starting time τ_0 ,

$$s(\mathbf{x}, \eta_s)|_{\tau=\tau_0} \propto f(T_A(\mathbf{x}), T_B(\mathbf{x})) \times g(T_A(\mathbf{x}), T_B(\mathbf{x}), \eta_s). \quad (2.21)$$

f is the entropy production at midrapidity as explain above. g parametrize the rapidity-dependence and is always normalized such that $g(\eta_s = 0) = 1$, so that it reduces to the original model at mid-rapidity. We parametrize the g function in terms of rapidity and then transformed to the space-time

rapidity.

$$g(\mathbf{x}, \eta) = g(y; T_A(\mathbf{x}), T_B(\mathbf{x})) \frac{J \cosh \eta_s}{\sqrt{1 + J^2 \sinh^2 \eta_s}}, \quad (2.22)$$

where the species-dependent factor J is replaced with an effective value $J \approx \langle p_T \rangle / \langle m_T \rangle$. To relate the asymmetry of $g(y)$ to the difference of T_A, T_B , we choose to parametrize the y -cumulents of g as functions of T_A and T_B . The $g(y)$ function is then reconstructed using its first few cumulants (mean μ , standard deviation σ , and skewness γ) by,

$$g(\mathbf{x}, y) = \mathcal{F}^{-1}\{\tilde{g}(\mathbf{x}, k)\}, \quad (2.23)$$

$$\log \tilde{g} = i\mu k - \frac{1}{2}\sigma^2 k^2 - \frac{1}{6}i\gamma\sigma^3 k^3 e^{-\frac{1}{2}\sigma^2 k^2} + \dots \quad (2.24)$$

where for the skewness term, we have included an exponential factor that systematically includes higher order cumulants to regulate the behavior of the function at large y . Numerically, we have found that within the range of $|y| < 3.3\sigma$, the reconstructed function has a good behavior and remains positive definite. The mean, standard deviation (width), and the skewness are parametrized as follows,

- For the mean parameter, we assume it is proportional to the center-of-mass rapidity of the local participant density $\mu = \mu_0 \eta_{\text{cm}}$,

$$\eta_{\text{cm}} = \frac{1}{2} \log \left[\frac{T_A e^{y_b} + T_B e^{-y_b}}{T_A e^{-y_b} + T_B e^{y_b}} \right] \quad (2.25)$$

where y_b is the beam rapidity.

- For the standard deviation, currently we leave it as a global parameter independent on the transverse location $\sigma = \sigma_0$, but only a function of the center-of-mass energy.
- For the skewness, there is not a preferred form, so we tested two parametrizations. And in the end, we will check whether the 3D initial condition extracted from data is sensitive to the different parametrizations schemes. These two choices are termed “relative skewness” and “absolute skewness”.
 - The “relative skewness” parametrization assume a skewness proportional to the relative difference of T_A and T_B ,

$$\mathcal{A}(T_A, T_B) = \gamma_r \frac{T_A - T_B}{T_A + T_B}, \quad (2.26)$$

Table 2.2 Table

Model	mean μ	std. σ	skewness γ
Relative	$\frac{1}{2}\mu_0 \ln \left(\frac{T_A e^{y_b} + T_B e^{-y_b}}{T_A e^{-y_b} + T_B e^{y_b}} \right)$	σ_0	$\gamma_r \frac{T_A - T_B}{T_A + T_B}$
Absolute	$\frac{1}{2}\mu_0 \ln \left(\frac{T_A e^{y_b} + T_B e^{-y_b}}{T_A e^{-y_b} + T_B e^{y_b}} \right)$	σ_0	$\gamma_a (T_A - T_B)/T_0$

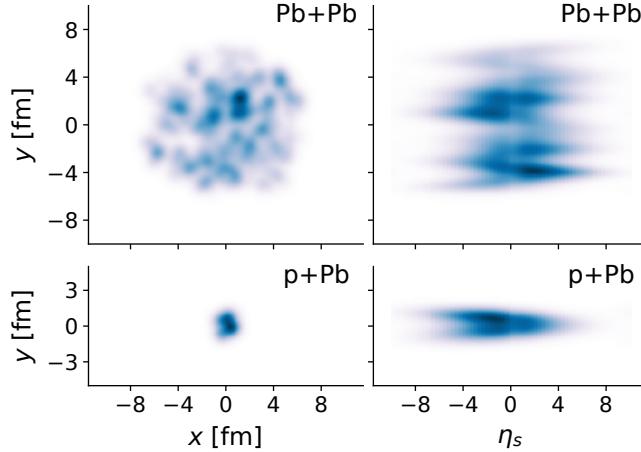


Figure 2.1 Two sample events for Pb+Pb collision (top row) and p+Pb collision (bottom row). The left column and the right column slice the initial entropy density at middle rapidity and the $x = 0$ plane respectively. The relative skewness parametrization is used with $\mu_0 = 1$, $\sigma_0 = 3$ and $\gamma_r = 6$.

- The “absolute skewness” parametrization assume a skewness proportional to the absolute difference of T_A and T_B ,

$$\mathcal{A}(T_A, T_B) = \gamma_a \frac{T_A - T_B}{T_0}. \quad (2.27)$$

And we put the unit for thickness function $T_0 = 1 \text{ fm}^{-2}$ to restore γ as a dimensionless parameter.

We have summarized the two parametrizations in table 2.2, and μ_0 , σ_0 , γ_r or γ_a , along with the effective Jacobian J are the four additional parameters one introduced for the three-dimensional extended TRENTOModel.

In figure 2.1, we show two sample events from a *Pb-Pb* collision (top plots) and a *p-Pb* collision (bottom plots) generated by TRENTOModel. The 3D

initial entropy densities are sliced at mid-rapidity $\eta_s = 0$ (left plots) and at the $x = 0$ plane (right plots). The mid-rapidity results are identical to the one predicted in the original T_RENTo model. The model is capable of generating fluctuating longitudinal structures that are local in the transverse plane, and breaks the boost-invariance both locally and globally. For the p -Pb event, there is a clear structure that one hot spot extends into the proton going side $\eta_s > 0$, while the participant clusters from the lead nuclei pushes the entropy production into the lead going side $\eta_s < 0$.

2.3 Reverse engineering the 3D initial condition

In the final section of this chapter, I apply the hydrodynamic-based simulation framework and the flexible T_RENTo-3D initial condition model to reverse engineer the 3D entropy deposition at the onset of hydrodynamics at the LHC energies.

Experimentally, one can only measure rapidity-dependent observables on an event averaged level, which already integrates the contribution of particle production over the transverse plane; while our parametrization in the T_RENTo model only involves local functions of the participant density function. So it is a nontrivial task to infer the functional form of local entropy production $s(\mathbf{x}, \eta_s)$ from these “global” measurements. The statistical technique for the reverse-engineering is the Bayes analysis explained in chapter 5.

2.3.1 Sensitive observables to the initial entropy deposition

The single particle spectra The most direct observable is the charged particle pseudo-rapidity density $dN_{\text{ch}}/d\eta$ measured for different collision systems and centralities. The ALICE collaboration and the ATLAS collaboration has measured this quantity for both Pb-Pb system ($-3.5 < \eta < 5.0$) and p-Pb system ($|\eta| < 2.7$). $dN_{\text{ch}}/d\eta$ can very well constrain the global rapidity profile and the centrality dependence of the mode, while the limitation being that it is less sensitive to the amount of longitudinal fluctuations.

Two particle pseudo-rapidity correlation A good probe of event-by-event longitudinal fluctuations is the two-particle pseudorapidity correlation observable $C(\eta_1, \eta_2)$,

$$C(\eta_1, \eta_2) = \frac{\langle N(\eta_1)N(\eta_2) \rangle}{\langle N(\eta_1) \rangle \langle N(\eta_2) \rangle} \quad (2.28)$$

The long range part of $C(\eta_1, \eta_2)$ is sensitive to initial state. This is because correlation between particles separated by a large rapidity gap at proper time τ can only come from proper time before $\tau e^{-|\eta_1 - \eta_2|/2}$ due to causality. For example, if two particles separated by four units of rapidity are emitted at a constant $\tau = 8 \text{ fm}/c$ hydrodynamic freeze-out hyper-surface and neglecting the long range correlation from the hadronic cascade, then any correlation must have come from before the proper time $8e^{-2} \approx 1 \text{ fm}/c$.

To see how $C(\eta_1, \eta_2)$ is related to the longitudinal fluctuation of the entropy deposition / particle production, decompose $dN_{\text{ch}}/d\eta$ for each event in a finite pseudo-rapidity window $[-Y, Y]$ using the normalized Legendre polynomials basis [49–51],

$$\frac{dN}{d\eta} = \left\langle \frac{dN}{d\eta} \right\rangle \left[1 + \sum_{n=0}^{\infty} a_n T_n \left(\frac{\eta}{Y} \right) \right], \quad (2.29)$$

$$T_n(x) = \sqrt{n + \frac{1}{2}} P_n(x) \quad (2.30)$$

Where $\langle \frac{dN}{d\eta} \rangle$ is the reference multiplicity at mid-rapidity for a certain centrality. a_0 is the total multiplicity fluctuation and a_1 controls how the multiplicity distribution is tilted in rapidity in each event and so on. Two-particle correlation $C(\eta_1, \eta_2)$ measures the variance of these a_n coefficients. Define the normalized event-wise distribution $R(\eta) = dN/d\eta/\langle dN/d\eta \rangle$, then the correlator is,

$$C(\eta_1, \eta_2) = \langle R(\eta_1)R(\eta_2) \rangle \quad (2.31)$$

$$= 1 + \sum_{m,n} \langle a_m a_n \rangle T_{mn}(\eta_1, \eta_2), \quad (2.32)$$

$$T_{mn}(\eta_1, \eta_2) = \frac{T_n(\eta_1)T_m(\eta_2) + T_m(\eta_1)T_n(\eta_2)}{2}. \quad (2.33)$$

Therefore, $\langle a_m a_n \rangle$ can be extracted by projecting the two particle correlation on to the function T_{mn} .

Combinations like $\langle a_0 a_n \rangle$ simply reflects how the event-wise rapidity fluctuation correlates with multiplicity fluctuation. These contribution is canceled to first order by another normalization to define C_N ,

$$C_N(\eta_1, \eta_2) = \frac{C(\eta_1, \eta_2)}{C_1(\eta_1)C_2(\eta_2)}, \quad (2.34)$$

$$C_{1,2}(\eta_{1,2}) = \int_{-Y}^Y C(\eta_1, \eta_2) \frac{d\eta_{2,1}}{2Y}. \quad (2.35)$$

Finally, C_N is directly related to the rapidity fluctuation it self,

$$C_N(\eta_1, \eta_2) \sim 1 + \frac{3}{2} \langle a_1^2 \rangle \frac{\eta_1 \eta_2}{Y^2} + \dots \quad (2.36)$$

We make use of the $\langle a_1^2 \rangle$ measurements to constrain the amount of linearly-tilting fluctuation in the initial condition model.

In additional to the initial condition fluctuation, short range correlation also contributes to the a_1 fluctuation [52]. The UrQMD hadronic afterburner is able to model certain type short range correlation coming from resonance decay and collisions, but jet-like correlations is hard to accounted for.

2.3.2 Calibration of the 3D initial condition parameters

The degrees of freedom of the initial condition model are,

- 1–2. Two normalization factors for Pb+Pb and p+Pb collisions at $\sqrt{s_{\text{NN}}} = 2.76$ TeV and 5.02 TeV beam energies. They are not fully independent as $N_{\text{p+Pb}} > N_{\text{Pb+Pb}}$ is always imposed in the parameter sweep.
- 3. The mid-rapidity entropy deposition parameter p .
- 4. The Γ -fluctuation variance parameter $1/k$.
- 5. The Gaussian nucleon width w , which determines initial state granularity.
- 6–8. Three coefficients that modulate the local rapidity distribution's shift μ_0 , width σ_0 , and skewness γ_r or γ_a ,
- 9. An average Jacobian J for the conversion from rapidity to pseudorapidity.

The range of the parameters is shown in 2.3. One may notice that we did not use different width parameters for the rapidity distribution σ_0 for $Pb+Pb$ and $p+Pb$ collisions, because the the beam rapidity changes less than 8% from 2.76 TeV to 5.02 TeV.

The dynamical model consists of a 3+1D relativistic hydrodynamics and a hadronic afterburner. The equation-of-state (EoS) is obtained by interpolating the state-of-the-art lattice-QCD EoS [53] at high temperature (zero baryon density) to a hadron resonance gas EoS at low temperature [54]. The energy density at which hydrodynamic energy momentum tensor is particulized into hadrons is $\epsilon_{sw} = 0.322$ GeV/fm³ corresponding to a switching temperature close to the pseudo-critical temperature $T_{sw} \sim T_c = 0.154$ GeV). As a remark, the relativistic hydrodynamics code

Table 2.3 Three-dimensional initial condition parameters

Parameter	Description	Range
N_{p+Pb}	Overall p+Pb normalization	140.0–190.0
N_{Pb+Pb}	Overall Pb+Pb normalization	150.0–200.0
p	Generalized mean parameter	-0.3–0.3 (with a prior)
k	Multiplicity fluct. shape	1.0–5.0
w	Gaussian nucleon width	0.4–0.6
μ_0	Rapidity shift mean coeff.	0.0–1.0
σ_0	Rapidity width std. coeff.	2.0–4.0
γ_0	Rapidity skewness coeff.	0.0–10.0 (rel) 0.0–3.6 (abs)
J	Pseudorapidity Jacobian param.	0.6–0.9

vHLLE [16] includes the viscous correction, but we used its ideal mode in the parameter extraction. This is because the parameter optimization process requires running the model on order hundreds different parameter sets. For each parameter set, thousands of minimum-biased events needed to be generated to control the statistical uncertainty, especially for the correlation observable. The full 3+1D viscous hydrodynamics is extremely time consuming, therefore we choose to ran the hydrodynamic model in its ideal mode and on a rather coarse grid. And the justification is that the rapidity distribution of the multiplicity and normalized two-particle correlations is less sensitive to the viscous effect. In the end, as a validation to this procedure, we will be using a set of high-likelihood parameter set and run the dynamical model with the viscous mode of the hydrodynamic mdoel to see if other observables such as the anisotropic flows, and event-plane decorrelations can be described.

Four thousands Pb+Pb and ten thousands $p+Pb$ events are generated at 100 set of parameter sets, then the Bayesian analysis makes inference on the probability distribution on the parameters by comparing to measurements. After the calibration, the $dN_{ch}/d\eta$ and a_1 fluctuation as function of centrality is compared to measurements in figure 2.2. The single particle distribution can be well reproduced by the calibrated initial condition plus dynamical evolution, while the correlation observables can be described upto 50% centrality. For more peripheral Pb+Pb collisions, the hydrodynamical based model significantly underestimate the a_1 fluctuation. We understand this as the consequence of inadequate modeling of the short range correlation for peripheral collisions, as they are more important in low multiplicity events

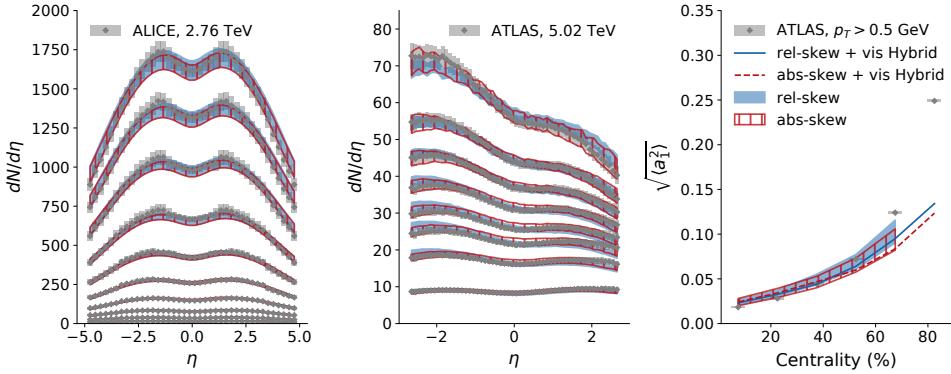


Figure 2.2 The posterior distribution of the observables after the fitting process. Blue and red stands for the results calibrated using the “relative skewness” and the “absolute skewness” ansatz respectively. From left to the right are charged particle pseudorapidity density in Pb+Pb collision, in p+Pb collision, and the rms of the a_1 coefficient in the two-particle pseudorapidity correlation decomposition. The lines in the right most figure shows that the rms a_1 is not very sensitive to the viscous effect in the hydrodynamic evolution.

($dN_{\text{ch}}/d\eta \sim 250$ and $N_{\text{part}} \sim 75$ at 50% centrality). In fact, the authors of [51] compared the measurements to the HIJING event generator that is based on mini-jet production. It is found that these jet-like correlations agrees well with the a_1 fluctuation for peripheral collisions with $N_{\text{part}} \lesssim 80$, while it overshoots the data for more central collision. The hydrodynamic model and mini-jet production model provide a complementary picture to fully understand the rms a_1 : at larger centrality, mini-jet production dominates the fluctuation of the $dN_{\text{ch}}/d\eta$, while as multiplicity increases and the final state interactions are so frequent and the event-by-event asymmetry in the single-particle distribution dominates rms a_1 .

Regarding the performances of different parametrization of the skewness, the “relative” skewness one does better in reproducing the uprising trend of rms a_1 , while the absolute skewness one better describes the large $dN_{\text{ch}}/d\eta$ asymmetry in the top 1% p+Pb collisions. However, there is no strong evidence to favor any of them over the other. We will see later that this is because the two parametrizations, though take different forms, actually behave similarly in terms of $ds/d\eta(\eta; T_A, T_B)$, for typical values of T_A and T_B of heavy nuclei.

The distribution of the calibrated parameters is shown in figure 2.3. The red and blue lines and color map correspond to results using the “absolute” and “relative” skewness respectively. The normalization parame-

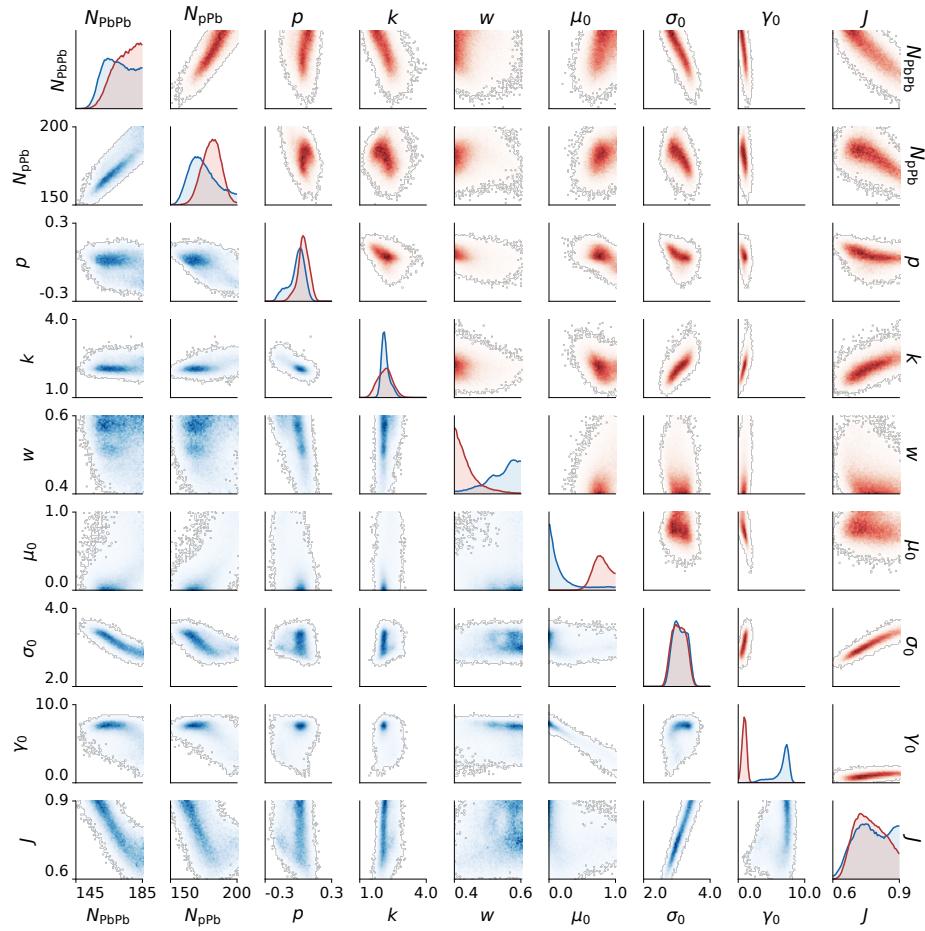


Figure 2.3 The posterior probability distribution of the model parameters, the colors distinguish the use of “absolute skewness” (red) and “relative skewness” ansatz. The diagonals are single parameter distribution, the off-diagonals are two-parameter joint distributions.

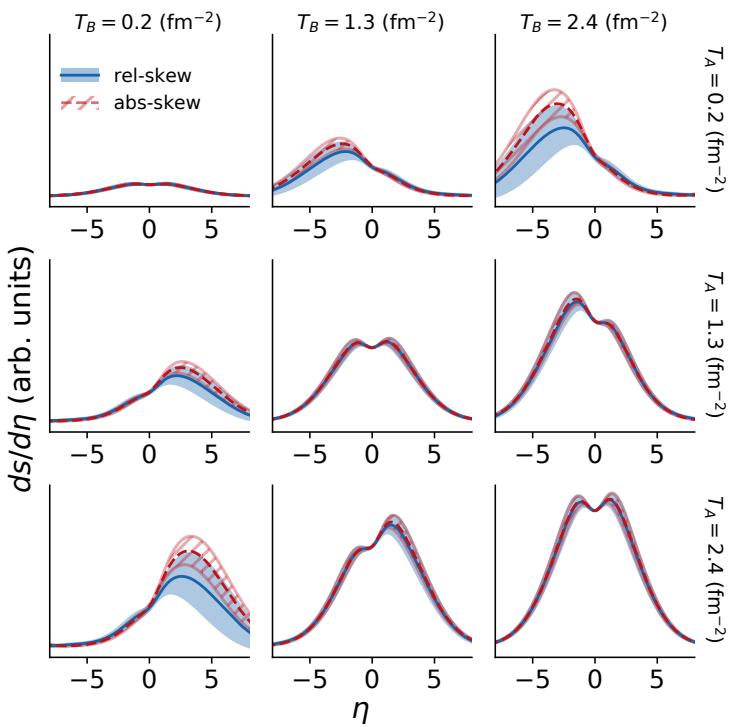


Figure 2.4 The constrained functional form of the three-dimensional initial entropy deposition $s(T_A(\mathbf{x}_\perp), T_B(\mathbf{x}_\perp), \eta_s)$. T_A and T_B is varied from 0.2 to 2.4 fm $^{-2}$. Colors distinguish the results from using “absolute skewness” (red) and “relative skewness” ansatz.

ters N_{PbPb} and N_{pPb} , mid-rapidity entropy deposition parameter p , nucleon thickness function fluctuation parameter k , the width of the rapidity distribution σ_0 and the effective Jacobian J have similar probability distributions between the two parametrizations. However, the distribution of the asymmetry related parameters μ_0 and γ_0 (anti-correlated), and nucleon width w are very different. This is because the Bayesian calibration looks for the high-likelihood region of the parameter space to explain the data, and the two different parametrizations can achieve this same goal by optimizing the parameter combinations differently. For the “relative” skewness one, the optimized parameters has a small shift of the mean μ and a large skewness γ ; for the “absolute” skewness one, it corresponds to the region with a large μ but vanishing γ . This does not mean that there are “two models” explaining the same data, because both of them are an oversimplified parametrization of $ds/d\eta(\eta; T_A, T_B)$ with infinitely many degrees of freedom. Instead, we should treat them as an estimation of the systematic uncertainty in extracting the function form of the initial 3D entropy deposition $ds/d\eta(\eta; T_A(\mathbf{x}), T_B(\mathbf{x}))$. It is more instructive to see the probability distribution of $ds/d\eta$ it self, given different values of $T_A(\mathbf{x})$ and $T_B(\mathbf{x})$. In Fig. 2.4, we samples the calibrated parameter distributions and use them to draw the entropy density as function of rapidity at different values of T_A and T_B . Again, the red and blue colors represents “absolute” and “relative” skewness parametrizations; the lines shows the median prediction and the bands are one standard deviation uncertainties. In each row and each column, T_A and T_B varies from 0.2 fm^{-2} to 2.4 fm^{-2} . For references, the value of the thickness function at the center of a Gaussian proton with nucleon width 0.5 fm is about 0.6 fm^{-2} and is 0.2 fm^{-2} at 1.5 width away from its center; while the maximum nuclear thickness function of a Pb nucleus is about 2.2 fm^{-2} . Therefore, the chosen range of $T_{A,B}$ already cover the typical ranges and combinations for entropy production in a realistic heavy-ion collision. One observe that the functional form of the ds/dy between the two parametrization agrees within one standard deviation, with the deviations increases as the asymmetry increases. Certainly, with a sufficient different T_A and T_B combination, the two results will have totally different predictions; however, within the physical range of the thickness function, the two methods converges onto a similar behavior. We conclude that by applying the hydrodynamic-based model and a flexible 3D initial condition, the form of the local rapidity distribution as function of participant densities can be reverse engineered using single particle pseudo-rapidity distribution and two-particle pseudo-rapidity correlation.

Table 2.4 A high likelihood parameter set

Parameter	rel-skew	abs-skew
$N_{\text{Pb+Pb}}$	150.0	154.0
p	0.0	0.0
k	2.0	2.0
w	0.59	0.42
μ_0	0.0	0.75
σ_0	2.9	2.9
γ_0	7.3	1.0
J	0.75	0.75

2.3.3 Prediction with the calibrated 3D initial condition

The calibrated initial condition is useful in predicting other rapidity-dependent observables. Especially, because we have only used multiplicities observables $dN_{\text{ch}}/d\eta$ and rms a_1 in the calibration, a prediction of azimuthal anisotropy related observables would provide an important validation of the initial condition. We choose a set of high-likelihood parameters showed in table 2.4. The selected validation / prediction observables are pseudo-rapidity dependent harmonic flows, event-plane decorrelations and the symmetric cumulants which quantifies the correlation between different flow harmonics.

Mid-rapidity v_n The elliptic and triangular flow from two-particle correlation $v_2\{2\}$ and $v_3\{2\}$ are calculated at as function of centrality at mid-rapidity (figure 2.5) and as function of pesudo-rapidity at different centrality (figure 2.6). We are able to describe flow measured by ALICE [55] at mid-rapidity with a shear viscosity $\eta/s = 0.17\text{--}0.19$ close to other phenomenological studies, though the bulk viscosity is not include in this study.

Rapidity-dependent v_n For the rapidity dependent flow figure 2.6, we used a larger $\eta/s = 0.25\text{--}0.28$. This inconsistency is because the ALICE measurement extrapolate p_T range for the rapidity-dependent flow down to 0, while the mid-rapidity p_T cut is $0.2 < p_T < 5.0$ GeV. It would not be a problem for the model to describe both with the same transport parameters, if the p_T differential flow and p_T differential particle spectra are both reproduced. However, due to the lack of a systematic tuning of the model parameters including both shear and bulk viscosity, the current mean p_T is too high. Therefore, agreement with the p_T -integrated flow in one kinematic cut does not guarantee the agreement to measurements that extrapolate to $p_T = 0$. Since our primary interest is the η -dependence of the flow, we have

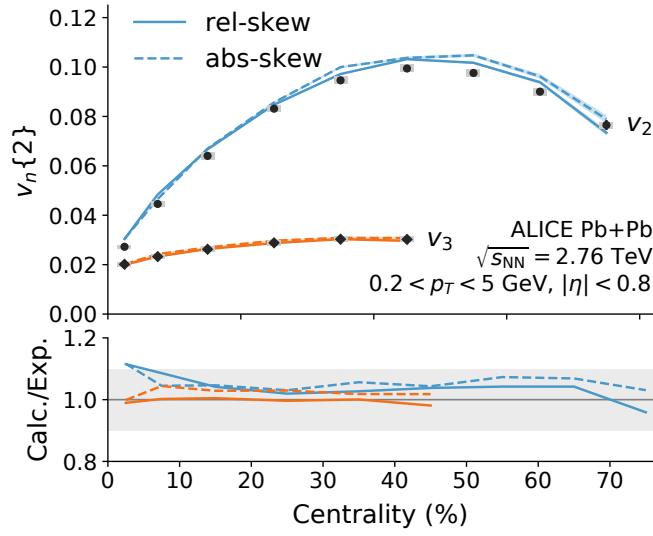


Figure 2.5 Flow coefficients $v_2\{2\}$ (blue) and $v_3\{2\}$ (orange) are plotted as a function of centrality. The calculation uses a 3+1D viscous hydrodynamic-based model with constant $\eta/s = 0.17$ and 0.19 for “relative skewness” (solid) and “absolute skewness” (dashed) ansatz. $\zeta/s = 0$ and the switching temperature is $T_{\text{sw}} = 154 \text{ MeV}$. The initial condition parameters are selected from the high-likelihood region of the posterior.

chosen this larger-than-usual shear viscosity to match the $v_2(\eta = 0)$ values to data. The calculated $v_2\{2\}$, $v_3\{2\}$, and $v_2\{4\}$ gradually decreases from mid-rapidity to forward / backward rapidity, which is also the trend of the data. The shape of $v_3\{2\}$ is well described; but for $v_2\{2\}$ and $v_2\{4\}$ in the region $|\eta| > 2.0$, the data decreases faster than our predictions. There could be several reasons for this differences. It is possible that the current initial condition model produce enough amount of fluctuation, but inadequate variance of the overlapping geometry as function of space-time rapidity. It is also showed in a study of at RHIC energies that the decreasing slope of $v_n(\eta)$ can be sensitive to the shear viscosity in the hadronic phase citeDenicol:2015bnf, Bozek:2010bi. But in our model, the transport properties of the system below T_c is all encoded in UrQMD and is not tunable. Moreover, we have assumed that hydrodynamization happens at a constant proper time hypersurface; while it is possible that a constant entropy density hypersurface is a better criteria, and as a result the matter at larger rapidity experiences a shorter period of pressure driven expansion. To systematically investigate all these effects, a future global parameter calibration including both initial condition parameters, transport parameters, and matching parameters is inevitable and is also feasible given the advance of the dynamical models and programming developments as well as more powerful computing resources.

Event-plane decorrelations The event-planes are defined as the phase angle of the anisotropic flow,

$$\Psi_n^{\text{EP}} = \frac{\text{atan}2(\langle \sin n\phi \rangle, \langle \cos n\phi \rangle)}{n}, \quad (2.37)$$

Due to longitudinal fluctuations, the event-planes separate by a rapidity gap decorrelates from each other. This decorrelation effect is important for observables that involves a large rapidity gap.

This event-plane decorrelation been studied using initial conditions from 3D extended Glauber model [57] and A Multi-Phase Transport (AMPT) model [58–60]. Recently developments such as solving the gluonic Yang-Mills dynamics in three-dimensions also studied the decorrelation of the initial eccentricity [42]. In our model, the geometry at forward and backward rapidity are dominated by the participants density of two different nuclei. And in between, the entropy production smoothly transit from one to another and so are the orientation of the energy density eccentricities that drives the flow of particles. The CMS collaborations quantifies the decorrelation by a

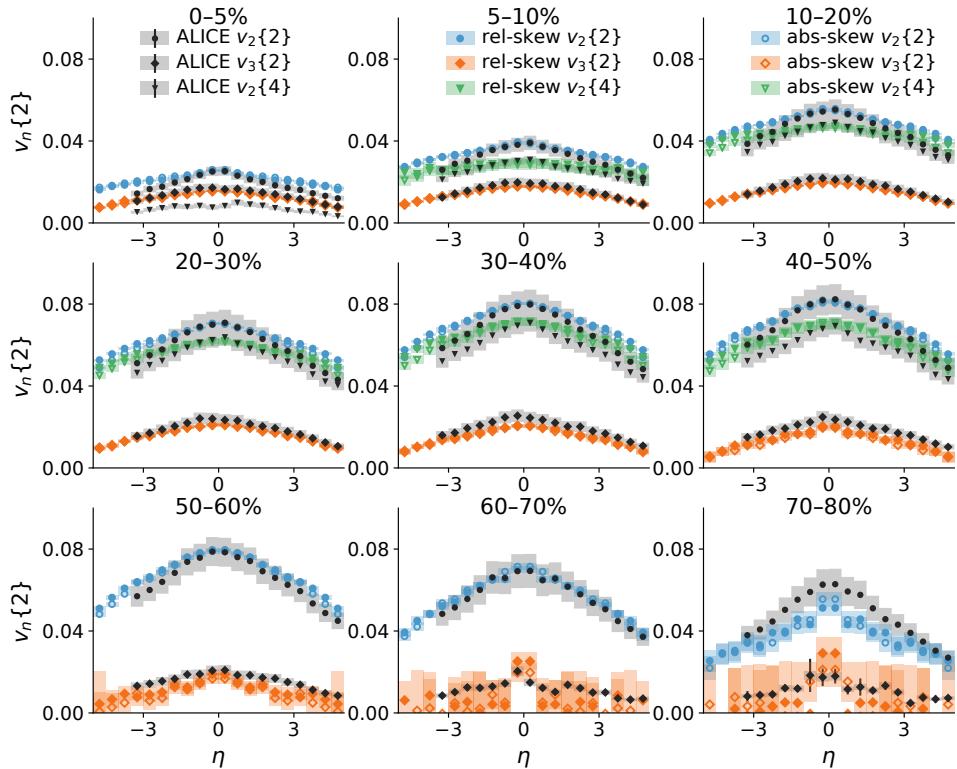


Figure 2.6 Pseudorapidity dependent flow coefficients $v_2\{2\}$ (blue circle), $v_3\{2\}$ (green triangle) and $v_2\{4\}$ (orange diamond). Constant $\eta/s = 0.25$ and 0.28 are used for “relative skewness” (closed symbol) and “absolute skewness” (open symbol) ansatz. Data is taken from the ALICE Collaboration [56].

three-bins factorization ratio [30],

$$r_n(\eta^a, \eta^b) = \frac{V_{n\Delta}(-\eta^a, \eta^b)}{V_{n\Delta}(\eta^a, \eta^b)}, \quad (2.38)$$

$$V_{n\Delta}(\eta^a, \eta^b) = \langle\langle \cos(n\Delta\phi) \rangle\rangle, \quad (2.39)$$

where the double average run over all particle pairs and all events. One of the rapidity bins is near η^b and the rest of the two bins are around $\pm\eta^a$. This ratio measures the decorrelation between two event planes separated by a larger rapidity gap $\eta^a + \eta^b$ relative to the decorrelation over a smaller gap $|\eta^a - \eta^b|$. In experiments, one would like take the reference bin η^b farther from η_a to suppress the short range correlations correlation. However, the way we build our model is to extend the mid-rapidity entropy deposition to finite rapidity, and this extension will eventually failed at sufficiently large rapidity because the model behavior in those region is not well constrained. In figure 2.7, we compare the model calculations to data with both a large $4.4 < \eta^b < 5.0$ (right) and a relative smaller $3.0 < \eta^b < 4.0$ (left). The predicted factoziation ratios decreases linearly with the the increasing rapidity gap. Using reference particles from $3.0 < \eta^b < 4.0$, the decorrelation is reproduced at larger centrality but not for central collisions. Because the $n = 2$ event-plane has a preferred direction defined by the impact parameter, while $n = 3$ event-plane does not, we observe that $n = 2$ factorization ratio decorrelates slower than the $n = 3$ ratio, except for the most central collision when $n = 2$ event-plane is also dominated by fluctuations. Comparing to data with reference particle from $4.4 < \eta^b < 5.0$, the experimental data stays similar to the the previous case except for central collisions, but the prediction is completely off. This is simply because the model fails on the details at large rapidity as we explained earlier. Given the present comparison, we conclude that the valid range of the model should be restricted to $|\eta| < 4.0$.

Symmetric cumulants Finally, we predict the symmetric cumulants (SC), which is a four particle correlation between different orders of anisotropic flows v_m and v_n [61, 62].

$$\begin{aligned} SC(m, n) &= \langle\langle \cos(m\phi_1 + n\phi_2 - m\phi_3 - n\phi_4) \rangle\rangle \\ &- \langle\langle \cos[m(\phi_1 - \phi_2)] \rangle\rangle \langle\langle \cos[n(\phi_1 - \phi_2)] \rangle\rangle \\ &= \langle v_m^2 v_n^2 \rangle - \langle v_m^2 \rangle \langle v_n^2 \rangle. \end{aligned} \quad (2.40)$$

It is clear from the second equation that it measures the covariance between v_n^2 and v_m^2 . One can also define the normalized symmetric cumulants (NSC),

$$NSC(m, n) = \frac{SC(m, n)}{\langle v_m^2 \rangle \langle v_n^2 \rangle}. \quad (2.41)$$

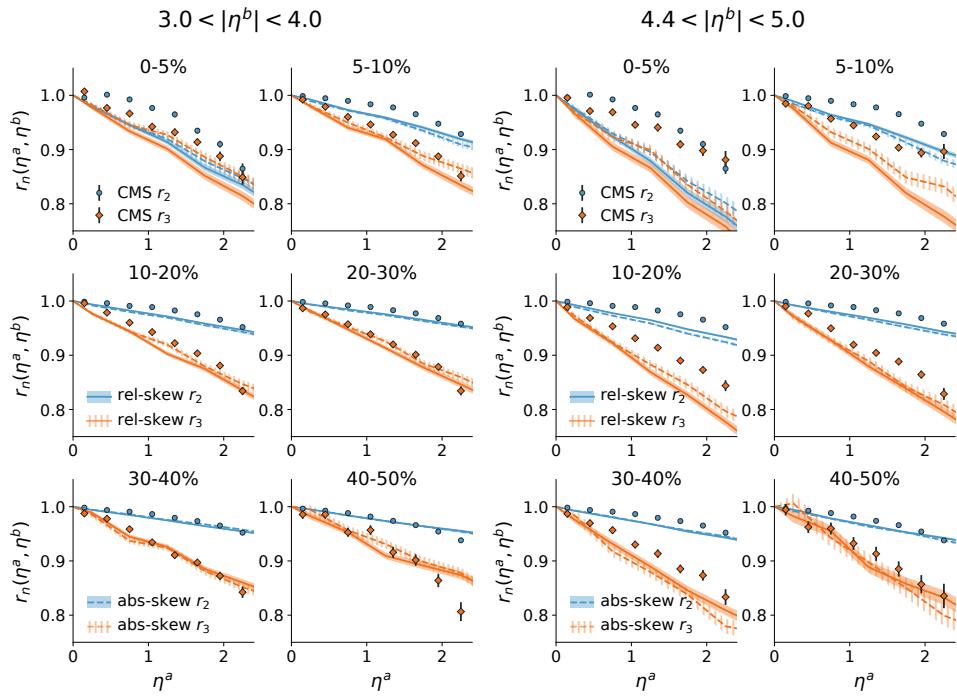


Figure 2.7 The $n = 2$ (blue) and $n = 3$ (orange) event-plane decorrelations obtained for “relative skewness” (lines with bands) and “absolute skewness” (lines with hatches) ansatz. The left and right plots uses different reference particle bins $3.0 < |\eta_b| < 4.0$ and $4.4 < |\eta_b| < 5.0$ respectively.

These observables are interesting because they are robust against flow effects, and have been shown to be sensitive to the temperature dependence of the transport coefficients [63]. Other analysis show that $SC(4, 2)$ probes the non-linear response of the hydrodynamic evolution, while $SC(3, 2)$ is more sensitive to initial conditions [64].

The relative- and absolute-skewness calculations are arranged on the left and right of 2.8. Symmetric cumulants $SC(4, 2)$ (blue) and $SC(3, 2)$ (green) are displayed in the top plots, and $NSC(4, 2)$ (blue) and $NSC(3, 2)$ (green) in the bottom plots. Within each plot, black dots are ALICE measurements at midrapidity $|\eta| < 0.8$ [63], which should be compared to the calculation shown in solid lines. The calculation shown in dashed lines are our predictions at forward/backward rapidity $2.5 < |\eta| < 3.5$,

$$\begin{aligned} SC'(m, n) = & \langle\langle \cos(m\phi_1 + n\phi_2 - m\phi'_3 - n\phi'_4) \rangle\rangle \\ & - \langle\langle \cos[m(\phi_1 - \phi'_2)] \rangle\rangle \langle\langle \cos[n(\phi_1 - \phi'_2)] \rangle\rangle, \end{aligned} \quad (2.42)$$

where the two of the particles (primed) are selected from the forward/backward rapidity bins, while the rest of the two still come from the mid-rapidity bin $|\eta| < 0.8$.

At mid-rapidity, the calculated (normalized) symmetric cumulants reproduce the trend of the measurements, and the “relative” skewed initial condition does a better quantitative job than the “absolute” skewed model. At forward and backward rapidity, though the magnitudes of both $SC(m, n)$ and v_n, v_m changed, the normalized symmetric cumulants remains the same as the one at mid-rapidity. This is a prediction that can be checked in future measurements to put further constraints on the three-dimensional initial condition model.

As a summary of this chapter, I have introduced the hydrodynamic-based medium evolution model that is very successful in describing the bulk observables. The sensitivity of the harmonic flows allows one to extract QCD transport coefficients using advanced statistical technique. The initial condition for the dynamical model is still a large source of uncertainty in both data interpretation and parameter extraction. The TRENTo model was developed as a flexible ansatz for mid-rapidity entropy / energy deposition so that the initial condition and interested transport coefficients can be calibrated simultaneously to data. Finally, I discussed my work on extending the TRENTo initial condition to include rapidity dependence and the use of multiplicity observable to reverse-engineer the functional form of initial 3D entropy deposition. The results can be used to predict more rapidity-dependent observables, and is useful to other studies involving a

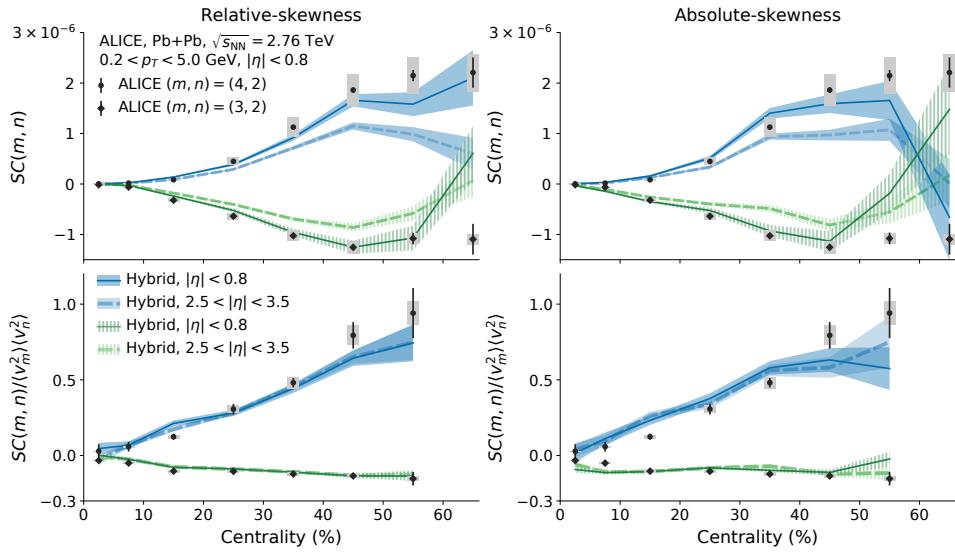


Figure 2.8 The symmetric cumulants (top row) and normalization symmetric cumulants (bottom row) obtained from the “relative skewness” (left column) and the “absolute skewness” (right column) ansatz. $SC(4, 2)$ (blue) and $SC(3, 2)$ (green) are shown as functions of centrality. The experimental measurements at middle rapidity ($|\eta| < 0.8$) are taken from [63]. The calculations are performed at both middle rapidity $|\eta| < 0.8$ (solid lines) and forward/backward rapidity $2.5 < |\eta| < 3.5$ (dashed lines).

large rapidity range. Due to the simplicity of the modeling, and the lack of global fit of all parameters including both 3D initial conditions and transport coefficients, we cannot yet answer how the inclusion of longitudinal fluctuation quantitatively affects the extracted QCD transport coefficients, but it is an important question for future precision analysis.

3

Transport model for hard partons in QGP

Hard partons are predominately created in perturbative scatterings at the earliest stage of relativistic heavy-ion collision. The distribution of the hard partons gets modified by the medium and the final final distribution carries information about the medium, as well as the hard-soft interaction properties.

Among the many ways of describing the in-medium evolution of hard partons, transport approach has its unique advantage. Here, we refer the transport approach to a class of models that evolve the semi-classical particle distribution function of hard partons in real time. Transport models can be often formulated as simulation on particle basis, which provides easy coupling to local properties of a dynamically evolving and fluctuating medium, and an exclusive final states. There are also challenges applying transport modeling in high energy collision. First, there are different assumptions of the interactions between the hard partons and the medium. Two commonly assumed extremes are:

- 1 A weakly coupled picture: medium consists of perturbative quasi-particles (scattering centers) whose distribution is close to local thermal equilibrium. Hard partons scatters pertrubtively with these well separated scattering centers. The dynamics are described by a Boltzmann equation.
- 2 Diffusion picture: interactions between the medium and the hard parton are frequent and soft, many body effects and non-perturbative effects can be important. The statistical effect of these interactions

are modeled by a drag and a diffusion coefficient. The dynamics is solved using a Langevin equation.

These two commonly used approaches are not necessarily mutually exclusive, and can have overlapped range of validity. For example, the effect of soft momentum exchange processes in the perturbative calculation can be very well modeled by a diffusion equation [65, 66]. These different assumptions on the interaction between the medium and the hard probe is largely due to our inadequate theoretical tools in describing the QGP medium in the strongly coupled regime. On the one hand, this becomes the model uncertain intrinsic to the transport approach, until one finds convincing way of interpreting the strongly coupled QGP medium from first principal. On the other hand, experiments may be able to tell which assumption (or a combination of both) is best and answers the very question of how the sQGP participates in the jet-medium interaction.

A second difficulty is that semi-classical transport equation can be cumbersome in treating of quantum coherence. Indeed, a quantum transition will always be bounded by the uncertainty principal: a process with momentum scale Q can not be localized within a space-time extend of $1/Q$. While in the semi-classical transport model, one always specify a local point in space-time where the interaction takes place. This is valid if the momentum scale Q is high enough that $1/Q$ is much smaller than the resolution that the transport model concerns, e.g., characterized by the mean-free-path in the Boltzmann equation. However, soft and collinear divergence of QCD bremsstrahlung (or more generally, parton branching and jointing) processes generate an abundance of small- Q events whose spatial extents can be much greater than the mean-free-path. This happens for certain phase space of the vacuum parton shower as well as the medium-induced parton shower. The vacuum parton shower are often solved as a vitality evolution with the time variable integrated out, while the transport equation is an evolution in time with virtuality integrated out, we shall postpone the discussions of their difference and matching to the next chapter. For medium-induced branching, this is the QCD analog of the Landau-Pomeranchuk-Migdal (LPM) effect [67–69], and the radiation pattern is changed qualitatively. When this happens, strictly speaking, the semi-classical transport equation is not the appropriate tool for these processes. However, considering the advantages of the transport formulation, we will develop a minimum set of modification to the semi-classical transport that can mimic some quantum effect of medium-induced branchings.

We start with an introduction of widely used transport equations: the

(linearized) Boltzmann equation and the Langevin equation. Next, taking elastic processes as example, we combine these two approach into a hybrid one by introducing a cut-off distinguishing hard and soft momentum transfer process following the idea in [65]. After that, we provide a brief review the theory of QCD in-medium parton branching processes at leading order, discussing its various approximations and also the numerical solutions in simplified medium. With these theoretical insights, the main progress of this chapter is developing a “modified Boltzmann” transport approach, treating the medium-induced parton branching with an approximate LPM effect. Finally, the simulations of the transport model are compared to the theoretical expectations to validate the implementation in different regime. We will show that the modified transport approach can reasonable describes the energy spectrum of the medium-induced splitting vertex for different channels $q \rightarrow q + g$, $g \rightarrow g + g$ and $g \rightarrow q + \bar{q}$. Treatment of the heavy quark masses effect, and running coupling are also investigated. For future references, in the very end, we make comparison between two other Monte-Carlo approach for medium-induced radiation with the present one and comment on the potential problems.

3.1 The Boltzmann equation

The Boltzmann equation evolves the transport of particles’ distribution function under the effect of localized collision. By localization, it means that the time scale of the collision has to be much smaller than the mean free-path $\tau \ll \lambda$. Therefore, the collision probability can be evaluated using local particle distribution function. It also allows one to include only few body collision processes, because the probability to interact with one more particle during this collision is small $P \approx \tau/\lambda \ll 1$. At weak coupling, we will see in the next section that this is indeed the case for elastic collision or soft and large angle radiation. But for radiation with a large formation time, its formation process becomes “non-local”. Accordingly, the Boltzmann formulation needed to be modified quite fundamentally for such processes. In this section, we only focus on local interactions.

With two-body to two-body (elastic) and two-body to three-body (inelastic, including the reverse process) processes, the Boltzmann equation for particle specie a takes the following form,

$$\frac{\partial f^a}{\partial t} + \vec{v} \cdot \frac{\partial f^a}{\partial \vec{x}} + \frac{\partial E}{\partial \vec{x}} \cdot \frac{\partial f^a}{\partial \vec{p}} = - \sum_{b,c,d} \mathcal{C}_a^{a+b \leftrightarrow c+d} - \sum_{b,c,d,e} \mathcal{C}_a^{a+b \leftrightarrow c+d+e} \quad (3.1)$$

On the left hand side, the distribution function $f^a(t, \vec{x}, p)$ undergoes transport with velocity $\vec{v} = \partial E / \partial \vec{p}$, and a possible potential potential force $\vec{f} = -\partial E / \partial \vec{x}$. On the right hand side of the equation, the $2 \leftrightarrow 2$ and $2 \leftrightarrow 3$ collision terms are functionals of the distribution functions. The summation of b, c, d, e iterates over all other particle species including a . Using the elastic process as an example and neglecting degeneracy of the internal quantum number for simplicity, the collision term can be separated into gain and loss terms,

$$\mathcal{C} = \mathcal{C}_{\text{loss}} + \mathcal{C}_{\text{gain}} \quad (3.2)$$

$$\begin{aligned} &= \int f^a(p_1) f^b(p_2) [1 + \epsilon^c f^c(p_3)] [1 + \epsilon^d f^d(p_4)] \overline{|M|^2}(p_1^a, p_2^b; p_3^c, p_4^d) d[PS]_{bcd} \\ &- \int f^c(p_3) f^d(p_4) [1 + \epsilon^a f^a(p_1)] [1 + \epsilon^b f^b(p_2)] \overline{|M|^2}(p_3^c, p_4^d; p_1^a, p_2^b) d[PS]_{bcd} \\ &= \int \left\{ f^a(p_1) f^b(p_2) [1 + \epsilon^c f^c(p_3)] [1 + \epsilon^d f^d(p_4)] \right. \\ &\quad \left. - f^c(p_3) f^d(p_4) [1 + \epsilon^a f^a(p_1)] [1 + \epsilon^b f^b(p_2)] \right\} \overline{|M|^2} d[PS]_{bcd} \end{aligned} \quad (3.4)$$

Where the crossing symmetry of the matrix-elements has been used in the last line of the equation $(\overline{|M|^2}(p_1^a, p_2^b; p_3^c, p_4^d) = \overline{|M|^2}(p_3^c, p_4^d; p_1^a, p_2^b) = \overline{|M|^2})$, and the phase-space integral is

$$d[PS]_{bcd} = \prod_{i \in b,c,d} \frac{dp_i^3}{2E_i(2\pi)^3} (2\pi)^4 \delta^4(p_1^a + p_2^b - p_3^c - p_4^d). \quad (3.5)$$

The $\epsilon = 0, -1, 1$ corresponds to classical, Fermi-Dirac, and Bose-Einstein statistics depending on the nature of the particle. The first term in the integration represents the loss of type- a particle in the phase-space around point (x, p_1) due to elastic collision, and the second term represents the gaining of type- a due to the reverse process. The symmetry in the microscopic matrix-element is very important for the kinetic equation to satisfy detailed balance: the probability to transition from one microscopic state to another equals that of the reverse process. The detailed balance ensures an thermal equilibrium limit of the system. Assume the system evolves long enough in a finite volume box and there is no spatial variance of the distribution function. Then the left of equation 3.4 is zero, and the static solution has to satisfy the relation,

$$f^a f^b (1 + \epsilon f^c) (1 + \epsilon f^d) = f^c f^d (1 + \epsilon f^a) (1 + \epsilon f^b), \quad (3.6)$$

for the entire phase-space and every combination of particle species. Therefore, the following combination is conserved for each reaction channel.

$$\frac{f^a}{(1 + \epsilon^a f^a)} \frac{f^b}{(1 + \epsilon^b f^b)} = \frac{f^c}{(1 + \epsilon^c f^c)} \frac{f^d}{(1 + \epsilon^d f^d)} \quad (3.7)$$

The available conservation quantities are the four momentum; therefore, one solution to the previous equation is,

$$\frac{f^a}{(1 + \epsilon^a f^a)} = e^{-\beta \mu_a - \beta p \cdot u} \quad (3.8)$$

for every particle species with parameters μ , β and a four vector u ($u^2 = 1$). So the static solution of the distribution is

$$f^a(p) = \frac{1}{e^{\beta \mu_a + \beta p \cdot u} - \epsilon^a} \quad (3.9)$$

$$\mu_a + \mu_b = \mu_c + \mu_d \quad (3.10)$$

The first line is the thermal distribution as expected that characterizes the kinetic equilibrium of the system, and the second line is the requirement for reaching chemical equilibrium. And one can identify the β and μ parameter as the inverse temperature and chemical potential. The u vector is the flow velocity of the cell as can be seen from the average velocity,

$$\left\langle \frac{p^\mu}{M} \right\rangle = \frac{\int f(p) \frac{p^\mu}{M} dp^3}{\int f(p) dp^3} = \frac{\int f(p) \frac{p^\mu}{M} dp^3}{\int f(p) dp^3} = u^\mu \quad (3.11)$$

3.1.1 The linearized Boltzmann equation and the diffusion limit

The full Boltzmann equations are many coupled differential-integral equations for each particle species. As a result, the analytic solutions for even simple form of interaction is almost impossible. The numerical solution / simulation is also a highly non-trivial task. However, under certain circumstances, a linearization of the Boltzmann equation is possible and greatly simplifies both analytic analysis as well as the numerical implementation.

The hard particles (jet partons, heavy flavors) are initially produced in perturbative processes with a large p_T or a large mass $M \gg T$. The perturbative production cross-section drops fast with the increase of p_T and m_T , so hard partons are very rare in an actual event. Therefore the occupation number of hard parton is a small number $f_H \ll 1$. One can neglect the

quantum statistics terms in the Boltzmann equation for them $1 + \epsilon f_H \approx 1$. For the Boltzmann equation of hard partons, the collision terms with more than one uncorrelated hard particles in the initial state can also be neglected since these contributions is proportional to $f_H^2 \ll f_H$. Finally, we also assume that the response of the bulk of the particles to the hard particles is small, and shall neglect any collision terms that involve a hard parton in the Boltzmann equation for the bulk distribution function (recently studies show that such back reactions is important to full jet observables, but we only consider leading particles in this thesis). Under these approximations, one arrived at a set of equations that is linearized with respect to the hard partons:

$$\frac{df_H}{dt} = -\mathcal{C}_H[f_H, f_{\text{bulk}}] \quad (3.12)$$

$$\frac{df_{\text{bulk}}}{dt} = -\mathcal{C}[f_{\text{bulk}}] \quad (3.13)$$

Here the collision term \mathcal{C}_H is linear with respect to f_H .

For the medium particles, the equations are still complex. However, a great simplification can be made by observing that the time it takes for the low momentum bulk particles to reach local thermalization is much shorter than the hard particles relaxation time, so a zeroth order approximation would be using the local thermal distribution 3.9. The space-time evolution of the temperature T , chemical potential μ and flow velocity u can be obtained from a hydrodynamic simulation that assumes the bulk medium stays close to local thermal equilibrium. Replacing the bulk medium distribution function by the thermal ones in 3.12, one arrives at a closed and linearized equation for the hard particles. Here we write down the equation assuming both the classical statistics and the conservation of the hard parton's species, and only elastic collision term is shown for simplicity,

$$\frac{df^H}{dt} = - \sum_b \int \left\{ f^H(p_1) f_{eq}^b(p_2) - f^H(p_3) f_{eq}^b(p_4) \right\} \overline{|M|^2} d[\text{PS}]_{234} \quad (3.14)$$

$$= - \int \left\{ f^H(p_1) w(p_1; p_3) - f^H(p_3) w(p_3, p_1) \right\} \frac{dp_3^3}{2E_3(2\pi)^3} \quad (3.15)$$

Where the $w(p; p')$ are the transition probability density for a particle with momentum p into momentum state p' ,

$$w(p; p') = \sum_b \int f_{eq}^b(p_2) \overline{|M|^2}(p, p_2; p', p_4) d[\text{PS}]_{24} \quad (3.16)$$

Using local thermal solutions for the bulk particles is a strong assumption. The degree of local thermalization in realistic events is still an open question, especially at early stage of the heavy-ion collision. Moreover, even if the system is close to its thermal limit, whether it can be understood in terms of the quasi-particle degrees of freedom using semi-classical distribution function is a different question. In an extreme weakly coupled system $g \ll 1$, one expected the local pressure and energy density can be explained in terms of the fundamental degrees of freedom: quarks and gluons, with perturbative corrections [70–72]. But with a large g estimated from phenomenology studies, such a perturbative description may not be most efficient way of understanding the bulk medium, and non-perturbative physics can play an essential role. Interpreting the medium in terms of microscopic degree-of-freedom seem to be a an unavoidable step of the Boltzmann equations, however, it is possible to “integrate out” the microscopic details in the soft limit of interaction into a set of transport coefficients.

The Fokker Planck equation In the soft momentum transfer $q = p' - p$ limit $|q| \ll |p|$, the change in distribution function can be expanded to the second terms in the q , and the linearized Boltzmann equation reduces to the Fokker-Planck type of equation,

$$\frac{df}{dt} = - \int \left\{ f(p) - \left[f(p) + \vec{q} \frac{\partial f}{\partial \vec{p}} + \frac{1}{2} \vec{q} \vec{q} \frac{\partial^2 f}{\partial \vec{p} \partial \vec{p}} \right] \right\} w(p', p) \frac{dp_3^3}{2E_3(2\pi)^3} \quad (3.17)$$

$$= - \int \left\{ \vec{q} \frac{\partial f}{\partial \vec{p}} - \frac{1}{2} \vec{q} \vec{q} \frac{\partial^2 f}{\partial \vec{p} \partial \vec{p}} \right\} w(p', p) \frac{dp_3^3}{2E_3(2\pi)^3} \quad (3.18)$$

$$= -\eta_D(p) \frac{\partial f}{\partial \vec{p}} + \frac{1}{2} B(p) \frac{\partial^2 f}{\partial \vec{p} \partial \vec{p}} \quad (3.19)$$

Where the vector function A and tensor function B are the first and second moments of the transition probability,

$$A_i(p) = \int w(p, p+q) q_i \frac{dp_3^3}{2E_3(2\pi)^3}, \quad (3.20)$$

$$B_{ij}(p) = \int w(p, p+q) q_i q_j \frac{dp_3^3}{2E_3(2\pi)^3}. \quad (3.21)$$

One remark is that although the form of the Fokker-Planck equation can be derived as the soft limit of the linearized version of the Boltzmann equation, its range of applicability is different from the later. This is because the transport coefficient is well defined in general regardless of whether one assumes quasi-particle type microscopic dynamics. In fact, in our final model,

we replace the soft sector of the Boltzmann equation with the Fokker-Planck equation so that the use of “medium quasi-particles” are restricted to hard momentum transfer processes. Moments beyond second order is dropped in deriving the Fokker-Planck equation, this is justified if the interaction is frequent enough so that within the smallest time scale that is concerned, there is already many interactions such that a statistical description of the effect of interaction is adequate in terms of the first (mean) and the second moments (variance). However, if the physical processes is rare, then fluctuation characterized by higher moments of the transition probability is very important and a diffusion approximation is not a good proxy.

Transport coefficients and Einstein relation The A and B function has to satisfy certain symmetry, as the only special direction after averaging over medium effects is the direction of motion. Therefore, $\vec{A} = \eta_D \vec{p}$ and it defines the drag coefficient η_D ; while the tensor B can be decomposed into a transverse part and a longitudinal part, with the respective transport coefficients κ and κ_L

$$B_{ij} = \kappa_L \frac{p_i p_j}{p^2} + \kappa \left(\delta_{ij} - \frac{p_i p_j}{p^2} \right) \quad (3.22)$$

One notice that medium temperature does not show up explicitly in the equation

$$\frac{df}{dt} = \frac{\partial}{\partial p_i} \left(\eta_D p_i + \frac{1}{2} \frac{\partial}{\partial p_j} B_{ij} \right) f \quad (3.23)$$

To guarantee the system has a thermalized solution, A , κ_{\parallel} and κ_{\perp} are not independent. Given a static and homogeneous medium at equilibrium with temperature T , $f = N \exp(-\beta E)$, the equation reduces to

$$0 = \frac{\partial}{\partial p_i} (\phi p_i f) \quad (3.24)$$

$$\phi = \eta_D - \frac{\kappa_{\parallel}}{2TE} + \frac{\partial \kappa_{\parallel}}{\partial p^2} + \frac{\kappa_{\parallel} - \kappa_{\perp}}{p^2}. \quad (3.25)$$

The Einstein relation $\phi = 0$ guarantees the exist of a equilibrium solution,

$$\eta_D = \frac{\kappa_{\parallel}}{2TE} - \frac{\partial \kappa_{\parallel}}{\partial p^2} - \frac{\kappa_{\parallel} - \kappa_{\perp}}{p^2} \quad (3.26)$$

This is where temperature shows up explicitly in the diffusion equation.

3.2 Hard parton transport in the incoherent limit

In this section, we shall first proceed using local and incoherent calculation of such processes and will discuss in great detail in the next section on including the LPM effect in a Boltzmann-like transport approach. The partonic processes are categorized into elastic (particle number conserving) and inelastic processes (particle number non-conserving). The inelastic processes are further divided into parton-splitting and parton-jointing contribution.

3.2.1 Hard/soft separation: elastic collisions

In a quasi-particle picture of the QGP, the hard parton collides with medium partons and transfer a certain amount of energy. These processes can be computed at leading order in the weakly coupled theory, where the collision cross-section is calculated using the dressed gluon propagator inside the medium [73],

$$D^{\mu\nu}(\omega, k) = \frac{\delta^{\mu 0}\delta^{\nu 0}}{k^2 - \Pi_L(\omega, k)} + \frac{\hat{P}_T^{\mu\nu}}{\omega^2 - k^2 - \Pi_T(\omega, k)} \quad (3.27)$$

where Π_T and Π_L are the self energies for transverse and longitudinal modes. Due to the presence of the medium, the dressed propagator lost its Lorentz invariance and depends on the complicated functions Π_T and Π_L . The resulting cross-section formula will be equally complicated. Fortunately, it has been shown recently in [65] that a simplification is possible at leading order in rewriting the elastic processes as large-angle scattering and small-angle diffusion. In such an approach, one chooses a scale Q_{cut} with a formal range of $gT \ll Q_{\text{cut}} \ll T$. For processes with momentum transfer to the medium larger than the cut-off (hard-mode) the medium screening effect is neglected and vacuum matrix-elements are used. While for processes smaller than the cut-off (soft-mode), the propagator receives significant contribution from the screen effect. The soft processes happen frequent and only involve small momentum transfer, satisfying the requirements of diffusion approximation. This separation allows the following modeling of the elastic interaction between hard parton and the medium,

$$\frac{df}{dt} = \mathcal{D}(Q_{\text{cut}})[f] + \mathcal{C}^{2\leftrightarrow 2}(Q_{\text{cut}})[f]. \quad (3.28)$$

So that the particle is continuously evolved by the diffusion process with its momentum occasionally changed by large-angle scatterings. Later we will verify that the cut-off dependence in the diffusion and scattering component

indeed cancels for “physical observations” at sufficiently small coupling. The phenomenological value of g is actually very large, so the residue cut-off dependence can be significant can there mag be significant non-perturbative contributionm, the merits of the current formulation is that certain non-perturbative effects can also be modeled by a diffusion processes with an additional contribution to \hat{q} .

Transport coefficients for soft modes The transverse and longitudinal diffusion constant below the cut-off has been calculated in [65],

$$\hat{q}_S = \int dq^2 \frac{\alpha_s m_D^2 T}{q^2(q^2 + m_D^2)} = g^2 C_R T m_D^2 \ln \left(1 + \frac{Q_{\text{cut}}^2}{m_D^2} \right). \quad (3.29)$$

$$\hat{q}_{S,L} = \int dq^2 \frac{\alpha_s m_\infty^2 T}{q^2(q^2 + m_\infty^2)} = g^2 C_R T m_\infty^2 \ln \left(1 + \frac{Q_{\text{cut}}^2}{m_\infty^2} \right) \quad (3.30)$$

$m_\infty^2 = m_D^2/2$ is the asymptotic gluon thermal mass. And the drag force is determined by the Einstein relation in equation 3.26,

$$\eta_D = \frac{\hat{q}_{S,L}}{2ET} - \frac{d\hat{q}_{S,L}}{dp^2} - \frac{2\hat{q}_{S,L} - 2\hat{q}_S}{2p^2} \quad (3.31)$$

Scattering rate for hard mode For the large- Q $2 \rightarrow 2$ scattering processes, the collision rates is computed by integrating the vacuum matrix-element,

$$R = \frac{d}{2E_1} \int \frac{d^3 p_2}{2E_2(2\pi)^3} f_0(p_2) 2\hat{s} \int_{-\hat{s}}^{Q_{\text{cut}}^2} \frac{d\sigma}{d\hat{t}} d\hat{t} \quad (3.32)$$

The integration is restricted to large momentum transfer above Q_{cut} and therefore we do not impose additional screening effect to regulate the matrix-element. In this work, the $2 \rightarrow 2$ matrix-element only includes the \hat{t} -channel contribution.

3.2.2 Hard/soft separation: inelastic collisions

The separation between hard and soft modes of the inelastic processes can also be performed similarly .

Diffusion induced branching For the incoherent diffusion-induced splitting rate, we borrow the expression from [74] while stripping the time-dependent phase factor,

$$R_{1 \rightarrow 2} = \int dk_\perp^2 dx \frac{\alpha_s P(x) \hat{q}_S(Q_{\text{cut}})}{2\pi(k_\perp^2 + m_\infty^2)^2} \quad (3.33)$$

where a gluon thermal mass is added to screen the divergence. Because these processes are induced by processes with medium momentum transfer below the cut-off, Q_{cut} appears in the formula. For the reverse processes $2 \rightarrow 1$ processes, similar reaction rate can be written down,

$$R_{2 \rightarrow 1} = \int e^{-\beta\omega} dk_{\perp}^2 dx \frac{\alpha_s P(x) \hat{q}_S(Q_{\text{cut}})}{2\pi(k_{\perp}^2 + m_{\infty}^2)^2} \quad (3.34)$$

where the rate is calculated in the rest frame of the medium. ω is the thermal parton's energy, and x is defined as the fraction of the thermal parton's energy to that of the final state hard parton.

Large- Q $2 \leftrightarrow 3$ process Regarding the $2 \rightarrow 3$ matrix-element, in previous study [75], we used to employ an improved version of the original Gunion-Bertsch cross-section that works under the limits $k_{\perp}, q_{\perp} \ll \sqrt{s}$ and $xq_{\perp} \ll k_{\perp}$ [76–78]. In the present study, we keep improving the matrix-elements by following the derivation in [77] while relaxing the condition $xq_{\perp} \ll k_{\perp}$. Therefore the updated matrix-elements contain the correct vacuum splitting function in the collinear limit. We summarize the matrix-elements here and have attached a derivation in the last section,

$$\overline{|M^2|}_{g+i \rightarrow g+g+i} = \overline{|M^2|}_{g+i \rightarrow g+i} P_{gg}^{g(0)} D_{gg}^g \quad (3.35)$$

$$\overline{|M^2|}_{g+i \rightarrow q+\bar{q}+i} = \frac{C_F d_F}{C_A d_A} \overline{|M^2|}_{g+i \rightarrow g+i} P_{q\bar{q}}^{g(0)} D_{q\bar{q}}^g \quad (3.36)$$

$$\overline{|M^2|}_{q+i \rightarrow q+g+i} = \overline{|M^2|}_{q+i \rightarrow q+i} P_{qg}^{q(0)} D_{qg}^q, \quad (3.37)$$

The two body matrix-elements that enters the $2 \rightarrow 3$ matrix-element is always required to be the t -channel contribution. $P_{bc}^{a(0)}(x)$ are vacuum splitting functions from parton a to partons b and c . Index i represent a quark / anti-quark or a gluon.

$$P_{gg}^{g(0)} = g^2 C_A \frac{1+x^4+(1-x)^4}{x(1-x)} \quad (3.38)$$

$$P_{qg}^{q(0)} = g^2 C_F \frac{1+(1-x)^4}{x} \quad (3.39)$$

$$P_{q\bar{q}}^{g(0)} = g^2 \frac{N_f}{2} (x^2 + (1-x)^4) \quad (3.40)$$

The D_{bc}^a contains the interference structure,

$$D_{qq}^g = C_A(\vec{a} - \vec{b})^2 + C_A(\vec{a} - \vec{b})^2 \quad (3.41)$$

$$\begin{aligned} D_{q\bar{q}}^g &= C_F(\vec{a} - \vec{b})^2 + C_F(\vec{a} - \vec{b})^2 \\ &\quad - (2C_F - C_A)(\vec{a} - \vec{b}) \cdot (\vec{a} - \vec{b}) \end{aligned} \quad (3.42)$$

$$\begin{aligned} D_{qg}^q &= C_F(\vec{c} - \vec{a})^2 + C_F(\vec{c} - \vec{b})^2 \\ &\quad - (2C_F - C_A)(\vec{c} - \vec{a}) \cdot (\vec{c} - \vec{b}) \end{aligned} \quad (3.43)$$

with the vectors given by

$$\vec{a} = \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2}; \vec{b} = \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2}; \vec{c} = \frac{\vec{k}_\perp}{\vec{k}_\perp^2}. \quad (3.44)$$

3.2.3 The final incoherent transport equation and Monte-Carlo technique

Combining all these processes, we summarize the incoherent linearized-Boltzmann plus Langevin equation into,

$$\frac{df}{dt} = \mathcal{D}[f] + \mathcal{C}_{1\leftrightarrow 2}[f] + \mathcal{C}_{2\leftrightarrow 2}[f] + \mathcal{C}_{2\leftrightarrow 3}[f]. \quad (3.45)$$

The distribution function of the hard parton undergoes soft diffusion and diffusion induced-radiation. Hard collision with the medium are included as $2 \leftrightarrow 2$ and $2 \leftrightarrow 3$ collision terms. The next section devotes to the inclusion of LPM effect to such an incoherent transport equation. At the end of this section, we present the numerical techniques for simulation the above equation.

The Monte Carlo method starts from representing the distribution function by an ensemble of particle states $\delta^3(x - x' - v(t - t'))\delta^3(p - p')$.

$$f(t, x, p) \approx \sum_i \delta^3(x - x_i(t))\delta^3(p - p_i(t)) \quad (3.46)$$

For linearized transport equations, it is sufficient to consider the dynamics of one such particle. Within a small time step δt , particles undergo scatterings with certainty probability. And then in between subsequent collisions, the particle is propagated by diffusion transport.

Order of operation In the presence of two types of operation: collision $\mathcal{C}[f_Q]$ and diffusion $\mathcal{D}[f_Q]$:

$$\frac{df}{dt} = (\hat{\mathcal{C}} + \hat{\mathcal{D}}) f_Q.$$

In principle, the order of operations on the particle should matter. But the difference choice of ordering only results in an $O(\Delta t^2)$ change in the updated distribution function. This can be seen with the formal solution of the equation,

$$\begin{aligned} f_Q(x, p) &= \exp \left\{ \int_{x'}^x \gamma u \cdot dx (\hat{\mathcal{C}} + \hat{\mathcal{D}}) \right\} f_Q(x', p) \\ &\approx e^{\Delta t \hat{\mathcal{C}}} e^{\Delta t \hat{\mathcal{D}}} f_Q(x', p) + \mathcal{O}(\Delta t^2) \end{aligned} \quad (3.47)$$

The diffusion solver The Fokker Planck equation can be solved as an ensemble of particles governed by the Langevin dynamics. The Langevin equation in the post-point discretization scheme is [79],

$$\Delta \vec{x}_i = \frac{p}{E} \Delta t \quad (3.48)$$

$$\Delta \vec{p}_i = -\Gamma \vec{p}_i \Delta t + \sqrt{\vec{B}(p + \Delta p) \Delta t} \vec{\xi} \quad (3.49)$$

Γ is the Langevin drag term, and $\vec{\xi}$ is a unit-variance Gaussian random force. $\vec{B} = \hat{P}^{\parallel} \kappa_{\parallel} + \hat{P}^{\perp} \kappa_{\perp}$ are the diffusion coefficients in the tensor form. \hat{P}^{\parallel} and \hat{P}^{\perp} projects any vector into the direction parallel and perpendicular to the direction of motion.

The diffusion coefficient are directly related to the one in the Fokker Planck equation $\kappa_{\parallel} = \hat{q}_L$, and $\kappa_{\perp} = \hat{q}/2$. While, the relation between the drag coefficient in the Fokker Planck equation η_D and the drag force Γ in the Langevin equation is discretization scheme dependent. In the post-step scheme, this relation is [79],

$$p_j \Gamma = p_j A + \left(\sqrt{\kappa_{\parallel}} \hat{P}_{lk}^{\parallel} + \sqrt{\kappa_{\perp}} \hat{P}_{lk}^{\perp} \right) \frac{\partial}{\partial p_l} \left(\sqrt{\kappa_{\parallel}} \hat{P}_{kj}^{\parallel} + \sqrt{\kappa_{\perp}} \hat{P}_{kj}^{\perp} \right). \quad (3.50)$$

and reduces to,

$$\Gamma = \eta_D + \frac{d\kappa_{\parallel}}{dp^2} + \frac{2\sqrt{\kappa_{\parallel}\kappa_{\perp}} - 2\kappa_{\perp}}{p^2} \quad (3.51)$$

$$= \frac{\kappa_{\parallel}}{2TE} - \frac{1}{p^2} \left(\sqrt{\kappa_{\parallel}} - \sqrt{\kappa_{\perp}} \right)^2. \quad (3.52)$$

The Einstein relation between η_D and diffusion coefficient is used in the last step.

The scattering solver For a two-body scattering, neglecting the quantum statistics, the collision rate in the rest frame of the medium is,

$$R_a(p) = \sum_{b,c,d} \frac{1}{2E_a} \int \frac{dp_b^3}{(2\pi)^3 2E_b} f_0(p_b) \int d\Phi_m |M^2|_{ab \rightarrow cd} \quad (3.53)$$

Similar expression can also be obtained for $2 \leftrightarrow 3$ processes. In a short amount of time Δt , the probability to have no collision is $P_0 = \exp(-\Delta t R)$. The number of independent multiple collisions satisfy a Poisson distribution with mean $N = \Delta t R$. For a particle based simulation, one always need to control δt small enough ($\Delta t \ll 1/R$) so that effectively there is at most one collision happens within the time step. Once a collision is sampled to happen, the full final states can be obtained by further sampling each scattering channel and the momentum phase-space differential rates.

The multi-dimensional phase-space sampling is performed sequentially for the initial state and final state phase-space. For $2 \rightarrow 2$ and $2 \rightarrow 3$ body processes, we rewrite the integrated rate in the fluid cell rest frame as,

$$R_{2m}(E_1, T) = \frac{d}{\nu} \frac{1}{2E_1} \int \frac{e^{-\beta E_2} dp_2^3}{(2\pi)^3 2E_2} \int d\Phi_m \overline{|M|^2}. \quad (3.54)$$

If vacuum matrix-element is used, the nested integration is a Lorentz invariant quantity, and we can choose to calculate it in the center-of-mass frame of the two-body collision,

$$\begin{aligned} \int d\Phi_m \overline{|M_{22}|^2} &= 2E_1 2E_2 v_{\text{rel}} \sigma \\ &= 2(s - M^2) \sigma_{\text{CoM}}^{22}(\sqrt{s}, T) \\ &= F_{2m}(\sqrt{s}, T) \end{aligned} \quad (3.55)$$

where σ is the cross-section of the process. In practice, the values of the integrated rates and cross-sections are tabulated. The sampling of initial state p_2 determines the center-of-mass energy of the process $s = (p_1 + p_2)^2 = 2(E_1 E_2 - p_1 p_2 \cos \theta_{12})$. Subsequently we sample the momentum-transfer q -differential cross-section with \sqrt{s}, T as inputs, and final states are reconstructed given the initial state and q . The sampling of $3 \rightarrow 2$ body process is more difficult due to the larger dimensional of parameters to specify the initial state kinematics,

$$R_{32}(E_1, T) = \frac{d}{\nu} \int \frac{e^{-\beta E_2} dp_2^3}{(2\pi)^3 2E_2} \frac{e^{-\beta k} dk^3}{(2\pi)^3 2k} \int d\Phi_2 \overline{|M|^2}. \quad (3.56)$$

The Lorentz invariant nested integral is a function of the initial 3-body state kinematics and temperature,

$$\int d\Phi_2 \overline{|M|^2} = F_{32}(\sqrt{s}, \sqrt{s_{12}}, \sqrt{s_{1k}}, T). \quad (3.57)$$

Where $s = (p_1 + p_2 + k)^2$ is the center of mass energy, $s_{12} = (p_1 + p_2)^2$ and $s_{1k} = (p_1 + k)^2$. This requires four-dimensional table for the value of F_{32} and a five-dimensional initial state sampling. The tabulation of a high-dimensional rate and cross-section tables can be made manageable if a proper approximating function $A(x, y, \dots)$ is proposed that captures the limiting behavior of the target function $T(x, y, \dots)$. Tabulating the ratio of T/A would be extremely efficient and accurate with a moderate size of the table.

The sequential sampling breaks the original $m + n$ body phase-space sampling into two lower dimension sampling. But as one should notice, the prerequisite is that the integration over the final state momentum of the matrix-element can be written into a Lorentz invariant form and therefore only depends on the Mandelstam variables. This appealing feature is certainly broken by the inclusion of either quantum statistics or in-medium propagator in the matrix-elements. Because quantum statistics introduces factors like $1 \pm f(p \cdot u)$ to the final momentum integral and the in-medium propagator is not Lorentz invariant, resulting in a F_{nm} that depends on the relative velocity between the collision system and the medium rest frame. This significantly increases the dimension and complexity of the problem. Fortunately, the separation of hard and soft mode showed in the last subsection allows one use vacuum matrix-element at large momentum transfer.

3.3 The Landau-Pomeranchuk-Migdal effect: theory

In the last section, all the processes are treated as instantaneous, however, a process actually takes a finite amount of time for its final states to loose coherence. For elastic collision, this time is $1/m_D \sim 1/gT$ which is still short compared to the mean-free-path $\lambda \sim 1/g^2 T$, provided a sufficiently small g . For inelastic process, the light-cone energy difference between the initial and final states is,

$$\delta E = \frac{k_\perp^2}{2k} + \frac{p_\perp^2}{2p} - \frac{p'^2_\perp}{2p'} = \frac{[(1-x)\vec{k}_\perp - x\vec{p}_\perp]^2}{2x(1-x)E} \quad (3.58)$$

By the uncertainty principal, the coherence time for such transition is on the order of $\tau_f = 1/\delta E$, termed the “formation time” of the radiation. Effects within the formation time should be calculated fully coherently. However, the formation time can be sufficiently long for collinear branching that it greatly exceeds the elastic collision mean-free path. This happens for small transverse momentum of the splitting that $k_\perp^2, p_\perp^2 < g^2 x(1-x)ET$. In this region of phase space, the average number of collision during the radiation becomes a relatively large number $N = \tau_f/\lambda > 1$, so the picture of independent radiation induced from independent scattering centers breaks down. It has been shown that these multiple scatterings should be resummed [69, 80, 81], and the leading order resummed radiation probability is,

$$\frac{dP_{bc}^a}{d\omega} = \frac{\alpha_s P_{bc}^{0,a}(x)}{x^2(1-x)^2E^2} \Re \int_0^\infty dt_1 \int_{t_1}^\infty dt_2 \nabla_{\mathbf{b}_1} \cdot \nabla_{\mathbf{b}_2} \{G(t_2, \mathbf{b}_2; t_1, \mathbf{b}_1) - G_0(t_2, \mathbf{b}_2; t_1, \mathbf{b}_1)\} |_{\mathbf{b}_1, \mathbf{b}_2 \rightarrow 0} \quad (3.59)$$

$P_{bc}^{0,a}(x)$ is the vacuum splitting function, and x is the energy fraction carried by the daughter b . Inside the double time intergal, G is the propagator of the following Hamiltonian for the transverse dynamics of the splitting system,

$$\hat{H} = \frac{-\nabla_{\mathbf{b}}^2 + m_{\text{eff}}^2}{2x(1-x)E} - i\Gamma_3(\mathbf{b}) \quad (3.60)$$

$$\Gamma_3(\mathbf{b}) = \frac{C_a - C_b + C_c}{2} \Gamma_2(\mathbf{b}) + \frac{C_a - C_c + C_b}{2} \Gamma_2(x\mathbf{b}) \quad (3.61)$$

$$+ \frac{C_b + C_c - C_a}{2} \Gamma_2((1-x)\mathbf{b}) \quad (3.62)$$

and G_0 is the free propagator. The variable \mathbf{b} is the Fourier transformation dual of the transverse momentum, and is usually referred as the impact-parameter (not to be confused with the other use). m_{eff}^2 is a combination of both parton bare masses and thermal masses. Finally, the interaction $\Gamma_3(\mathbf{b})$ encodes the transverse broadening of the three body system $a \rightarrow b+c$ [80]. It has three pieces of two-body contributions $\Gamma_2(\mathbf{b})$. The vacuum pieces G_0 is subtracted from G so that this formula only computes the medium-induced radiation. The two gradient operators at time t_1 and t_2 come from the action of the radiation vertices, meaning this transition receives coherence contribution from t_1 to t_2 . If one neglects the mass term, G can be rewrite

as $G_0 - iG_0\Gamma_3G$ so that,

$$\frac{dP_{bc}^a}{d\omega} = \frac{\alpha_s P_{bc}^{0,a}(x)}{x^2(1-x)^2 E^2} \Re e \int_0^\infty dt_1 \int_{t_1}^\infty dt_2 \nabla_{\mathbf{b}_1} \cdot \nabla_{\mathbf{b}_2} [G_0(-i\Gamma_3)G](t_2, \mathbf{b}_2; t_1, \mathbf{b}_1) |_{\mathbf{b}_1, \mathbf{b}_2 \rightarrow 0} \quad (3.63)$$

$$= \frac{\alpha_s P_{bc}^{0,a}(x)}{x^2(1-x)^2 E^2} \Re e \int_0^\infty dt_1 \int_{t_1}^\infty dt_2 F(t_2; t_1) \quad (3.64)$$

And $F(t_2, t_1)$ is a short notation for term under the integration.

The interaction potential $\Gamma_2(\mathbf{b})$ really depends on the assumption of the probe-medium interaction. For example, in a weakly coupled theory, a quite compact results is obtained at leading order [82],

$$\Gamma_2(\mathbf{b}) = \frac{1}{\pi} \int \frac{d\mathbf{q}_\perp^2}{(2\pi)^2} \frac{g^2 T m_D^2 (1 - e^{i\mathbf{b} \cdot \mathbf{q}_\perp})}{q_\perp^2 (q_\perp^2 + m_D^2)} \quad (3.65)$$

There are two systematic ways to investigate the properties of the medium-induced radiation computation. The first method is called the opacity expansion [83, 84], which amounts to solve the propagator in a perturbation series of the number of interaction Γ_3 . Another approach which studies the solution assuming soft interaction (small- q) and approximate the collision kernel by a harmonic oscillator one $\Gamma_2(b) \approx \frac{1}{4}\hat{q}b^2$ [81, 85, 86]. This is also known as the leading-log $1/\ln(N)$ approximation, where N can be understood as the “number” of coherent collision within the formation time. Taking the residue potential $\Gamma(b) - \frac{1}{4}\hat{q}b^2$ as a perturbation, improvements at the next-to-leading-log level has also been investigated in [87, 88].

Though this leading order calculation has been written in this compact form, it is not trivial to include its effect (even approximately) in the semi-classical Boltzmann simulation. One can also see this problem more evidently by observing that it requires a finite time interval $t_1 \rightarrow t_2$ to compute the splitting rate at time t_1 , while Boltzmann equation has only one time variable in the . We will devote the next section to an approximation solution to this problem. For the rest of this section, we shall elaborate the details of the current understanding in the opacity expansion and harmonic oscillator (deep-LPM) regime, which greatly facilitate the discussion of the next section.

3.3.1 Large medium

For a large and static medium that approaches the infinite medium limit. Further simplification is possible that the calculation of the transition probability becomes a “static” problem, and a branching rate Γ can be defined

as the branching probability per unit time. This limit is known as the AMY formalism [89–91],

$$\frac{d\Gamma_{a \rightarrow bc}}{dx} = \frac{1}{2E\nu_a} \frac{\alpha_s d_a P_{a \rightarrow bc}(x)}{x^2(1-x)^2} \int \frac{d^2\vec{k}}{(2\pi)^2} \vec{k} \cdot \Re e \vec{F}$$

where we have dropped the Bose enhancement and the Pauli blocking factors of the outgoing partons from the original formula. The vector valued wavefunction $\vec{F}(\vec{h}; p, x)$ satisfies the following integral equation [89],

$$2\vec{k} = i \frac{\vec{F}(\vec{k})}{\tau_f(k)} + g^2 \mathcal{C}_3[\vec{F}]$$

\vec{k} , and $\tau_f(k)$ is the transverse scale and the formation time of the branching. \mathcal{C}_3 is the Γ_3 operator in the momentum representation,

$$\begin{aligned} \mathcal{C}_3[f] &= \int_{\mathbf{q}} \mathcal{A}(q_\perp^2) \left\{ \frac{C_b + C_c - C_a}{2} (f_{\mathbf{p}} - f_{\mathbf{p}-\mathbf{q}}) \right. \\ &\quad \left. + \frac{C_a + C_c - C_b}{2} (f_{\mathbf{p}} - f_{\mathbf{p}+x\mathbf{q}}) + \frac{C_a + C_b - C_c}{2} (f_{\mathbf{p}} - f_{\mathbf{p}+(1-x)\mathbf{q}}) \right\} \end{aligned} \quad (3.66)$$

$$\mathcal{A}(q_\perp^2) = \frac{g^2 m_D^2 T}{q^2 (m_D^2 + q^2)} \quad (3.67)$$

The exact solution can be solved numerically. Here, we build the understanding of this formula in two extreme regimes: the incoherent limit (Bethe-Heitler regime) and the deep-LPM regime.

The Bethe-Heitler regime: The quantum interference can be neglected if the formation time is sufficiently short. In such cases the amplitude under the double time integral has a delta-function like time structure, and the transition probability has a nice interpretation of integrating localized branching rate over a single time variable. But the kinematic range for short enough formation time is very limited. The condition $\tau_f \ll \lambda$ translates to $\omega \ll T$. For such case, one may solve for F by treating F/τ_f as a large quantity [65]. The leading equations are then,

$$2\vec{k}\tau_f(k) = -\Im m \vec{F} \quad (3.68)$$

$$\Re e \vec{F} = -g^2 \tau_f(k) \mathcal{C}[\Im m \vec{F}] \quad (3.69)$$

Take quark splitting into a quark and a gluon as an example and neglecting the thermal masses, the resulting rate is then proportional to

$$R \propto 2g^2 \int dk^2 \int dq^2 \mathcal{A}(q_\perp^2) \left\{ \frac{C_A}{2} \frac{\vec{k}}{\vec{k}^2} \cdot \left[\frac{\vec{k}}{\vec{k}^2} - \frac{\vec{k} - \vec{q}}{(\vec{k} - \vec{q})^2} \right] + \frac{2C_F - C_A}{2} \frac{\vec{k}}{\vec{k}^2} \cdot \left[\frac{\vec{k}}{\vec{k}^2} - \frac{\vec{k} + x\vec{q}}{(\vec{k} + x\vec{q})^2} \right] + \frac{C_A}{2} \frac{\vec{k}}{\vec{k}^2} \cdot \left[\frac{\vec{k}}{\vec{k}^2} - \frac{\vec{k} + (1-x)\vec{q}}{(\vec{k} + (1-x)\vec{q})^2} \right] \right\} \quad (3.70)$$

though, this expression looks very different from the cross-section formula that we used in the incoherent rate in the Boltzmann equation, they are actually equivalent upon the integration of dk^2 , we provide detailed explanation of this connection between the Bethe-Heitler approximation of the AMY rate equation and the incoherent rate computed with $2 \rightarrow 3$ cross-section in section 3.7.

In the high energy limit $E \gg T \gg \omega$ so that $x \ll 1$, this rate can be approximated by its $x \rightarrow 0$ limit,

$$\begin{aligned} \frac{dR}{dx} &= \frac{4E\alpha_s d_a P(x)}{\nu_a} \int \frac{dk^2}{(2\pi)^2} \int \frac{dq^2 \mathcal{A}(q_\perp^2)}{(2\pi)^2} \sum_{\pm} \frac{C_A}{2} \frac{\vec{k}}{\vec{k}^2} \cdot \left[\frac{\vec{k}}{\vec{k}^2} - \frac{\vec{k} \pm \vec{q}}{(\vec{k} \pm \vec{q})^2} \right] \\ &= \frac{2C_A E \alpha_s d_a P(x)}{\nu_a} \int \frac{dk^2}{(2\pi)^2} \int \frac{dq^2 \mathcal{A}(q_\perp^2)}{(2\pi)^2} \left[\frac{\vec{k}}{\vec{k}^2} - \frac{(\vec{k} - \vec{q})}{(\vec{k} - \vec{q})^2} \right]^2 \quad (3.72) \end{aligned}$$

where in the second step, the k integration of the term with the "+" sign has been shifted to an integration over $k - q$ to render the expression into the completing square form. This form is known as the Gunion-Bertsch approximation [76] of inelastic $2 \rightarrow 3$ scattering, whose improved form [77, 78] has been employed in existing full Boltzmann simulation of partonic transport equation [92, 93]. To understand the physical meaning of the above expression, we can proceed to integrate and regulate soft divergence with a screening masses whenever needed. Eventually we have,

$$\frac{dR}{dx} \propto \alpha_s P(x) \times \alpha_s C_A T \propto \frac{\alpha_s P(x)}{\lambda_g} \quad (3.73)$$

Where the second factor $\alpha_s C_A T$ can be interpreted as the inverse of gluon-mean-free path. Now the physical meaning becomes clear: in the incoherent limit, certain amount of radiation $\alpha_s P(x)$ is triggered every mean-free-path from interaction with the collision centers.

To summarize in the Bethe-Heitler regime, the total number of branching can be viewed as contributed by a incoherent sum $2 \rightarrow 3$ processes localized at time t . And such contribution can be easily incorporated into the

Boltzmann equation given the incoherent branching rate. However, the valid range for this approximation is at best $xE \sim$ a few times of the temperature.

The deep-LPM region (leading-log behavior): another useful approximation considers the limit τ_f is so large that many collisions contribute coherently to the branching. This corresponds to those energetic split $\omega \gg T$. As a result, the transverse momentum k of the branching should be large compared to the average momentum transfer to each scattering centers q . In this limit, a diffusion approximation to the \mathcal{C} operators is possible. The finite difference between $F(k)$ and $F(k+O(q))$ is expanded in \vec{q} . The zeroth order cancels and the first order \vec{q} contribution vanishes due to the symmetric q integration. Keeping only second order terms in \vec{q} , the AMY equation is simplified to a diffusion type equation but with complex diffusion constant and a source term [87]

$$-\frac{1}{4}\nabla_{\vec{k}}^2 \vec{F} + i\frac{k^2 + m_{\text{eff}}^2}{2x(1-x)E\hat{q}_3} \vec{F} = \frac{2\vec{k}}{\hat{q}_3}. \quad (3.74)$$

This approximation of the original collision operator is also known as the harmonic oscillator approximation, because in the impact-parameter space, this approximation leads to a quadratic form of $\Gamma_2 \propto b^2$. Finally, \hat{q}_3 is the effective transport parameter for conveniences

$$\hat{q}_3(x, Q_0^2) = \alpha_s T m_D^2 \ln \left(1 + \frac{Q_0^2}{m_D^2} \right) C_{abc}(x). \quad (3.75)$$

This is obtained by doing the \mathbf{q} integration of the expanded collision operator upto a cut-off scale Q_0 , below which the small- q approximation is considered to be valid. The effective transport parameter also depends on the color structure of the splitting,

$$C_{abc}(x) = \frac{C_b + C_c - C_a}{2} + x^2 \frac{C_a + C_c - C_b}{2} \quad (3.76)$$

$$+ (1-x)^2 \frac{C_a + C_b - C_c}{2} \quad (3.77)$$

Taking the momentum fraction of the “ b ” particle to zero $x \rightarrow 0$, this color factor goes to C_b ; similarly, $x \rightarrow 1$ which corresponds to “ c ” particle taking vanishing fraction of the total energy, the color factor approaches C_c . Therefore, in these extreme limits $x \rightarrow 0$ or 1 , the effect transport parameters looks like the daughter with softer momentum. With finite $x, 1-x$, the color factor becomes a combination of the colors of the whole splitting system.

Neglecting the thermal mass, the solution to the this diffusion equation can be obtained analytically [87],

$$\vec{F} = i4x(1-x)E^2 \frac{\vec{k}}{k^2} \left[\exp\left(\frac{-i^{1/2}k^2}{\sqrt{2x(1-x)E\hat{q}_3}}\right) - 1 \right] \quad (3.78)$$

And the radiation rate can be obtained accordingly,

$$\frac{dR_{bc}^{a,\text{LL}}}{dx} = \frac{\alpha_s P_{bc}^{a(0)}}{\pi\sqrt{2}} \sqrt{\frac{\hat{q}_3(x, Q_0^2)}{2x(1-x)E}} \propto \frac{\alpha_s P(x)}{\langle\tau_f\rangle} \quad (3.79)$$

Such a result is often referred to as the leading-log solution, because it is an expansion in terms of $1/\ln(N)$ with N the “number” of coherent collision centers. An interesting scale $\sqrt{2x(1-x)E\hat{q}_3}$ shows up in such calculation which governs the typical transverse momentum of the splitting, or equivalently $\sqrt{\hat{q}_3/2x(1-x)E}$ which governs the rate at which the splitting happens. A simple interpretation for these scales is: during $\tau_f \sim 2x(1-x)E/k_\perp^2$, many soft interactions contribute to the broadening of k_\perp^2 . In a diffusion approximation, the variance $\langle k_\perp^2 \rangle$ is linearly proportional to the diffusion constant and time, $\langle k^2 \rangle \sim \hat{q}_3\tau_f$. Combining with the expression of formation time, one arrives at the above typical transverse momentum and typical formation time.

Compared to the naïve “incoherent expectation”, the actual radiation rate is reduced by a factor of $\lambda_{\text{el}}/\langle\tau_f\rangle$ on average. Therefore, in the deep-LPM regime, instead of triggering radiation every mean-free-path, a large collision centers contribute coherently and trigger radiation every τ_f which scales as $\lambda\sqrt{\omega/T}$. Considering that this approximation only works for $\omega \gg T$, we combine this result with the Bethe-Heitler regime and summarize the radiation pattern in a large medium as,

$$\frac{dR_{bc}^a}{dx} \sim \frac{\alpha_s P_{bc}^{a(0)}(x)}{\max\{\lambda, \tau_f\}} \quad (3.80)$$

This simple idea will be the foundation for developing the transport modeling of the parton branching processes in the section section.

The deep-LPM region (next-to-leading-log level): The previously introduced leading-log result has both a charming simplicity and a clear physical interpretation in explaining what happens in the deep-LPM region $\ln(N) \sim \ln(xE/T) \gg 1$. Together with the Bethe-Heitler (incoherent) limit at $xE \lesssim T$, one can already build a pretty good understanding in an infinite medium.

One thing that still deserves a detailed discussion is the upper bound Q_0 introduced to the q -integration in the leading-log approximation. This cut-off scale, as a result of the small- q simplification of the full model, is generally unknown and brings an uncertainty to the approximation at this level. And we need better understanding to build a good transport model proxy of the underlying theory. This issue has been studied at the next-to-leading-log (NLL) level by treating the large- q part of the collision kernel as a perturbation to this approximation, authors of [87] and more recently by authors of [88] had found that reasonable choice of Q_0 is the order of k_\perp^2 itself. A self-consistent determination of Q_0 is also possible by requiring a minimal contribution from the NLL correction. The NLL results, takes a similar structure of the leading-log solution, but with the unknown Q_0 replaced by its NLL improvements Q_1 ,

$$Q_1^2 \approx \sqrt{\omega \hat{q}} \approx \sqrt{\omega \alpha_s C_R m_D^2 T \ln \frac{Q_0^2}{m_D^2}} \quad (3.81)$$

or a self-consistent determination as in [87],

$$\begin{aligned} Q_1^2 &= \sqrt{2x(1-x)E\alpha_s T m_D^2} \\ &\times \left(\frac{C_b + C_c - C_a}{2} \ln \frac{2\xi Q_1^2}{m_D^2} + \frac{C_a + C_c - C_b}{2} x^2 \ln \frac{2\xi Q_1^2}{x^2 m_D^2} \right. \\ &\left. + \frac{C_a + C_b - C_c}{2} (1-x)^2 \ln \frac{2\xi Q_1^2}{(1-x)^2 m_D^2} \right)^{1/2} \end{aligned} \quad (3.82)$$

with $\xi \approx 9.1$ a constant. This suggests that the optimal choice of the scale is on the branching transverse momentum itself $\langle k^2 \rangle = \sqrt{2x(1-x)E\hat{q}_3}$, but with an improved logarithmic factor. It has been shown that using this self-consistent Q_1 brings the approximation very close to the numerical solution of the full model when $\omega \gg T$. In the next section, we shall also make use of this NLL solution to validate the performance of the transport simulation.

3.3.2 Thin medium: opacity expansion

The realistic medium created in a heavy-ion collision are always finite and expanding. Whether the medium is large enough for a certain branching should be determined by the comparison of the formation time and the size of the medium (or the expansion time scale). For thin and dilute medium,

there is only a few effective collision that contributes. In such cases, systematic expansion over L/λ has been developed can is known as the opacity expansion. This can be obtained by solving the propagator with an perturbation series of the interaction potential Γ_3 . At leading order in the opacity expansion and apply soft approximation $x \ll 1$, the radiation rate is [94],

$$\frac{dR}{dx} \propto g^2 P(x) C_A \int \frac{d\vec{q}^2 d\vec{k}}{(2\pi)^4} \frac{g^2 T m_D^2}{q^2(q^2 + m_D^2)} \frac{\vec{k} \cdot \vec{q}}{(\vec{k} - \vec{q})^2 k^2} \left[1 - \cos \left(\frac{(\vec{k} - \vec{q})^2 t}{2xE} \right) \right] \quad (3.83)$$

It has a notable time-dependent $1 - \cos(\omega t)$ modulation due to interference from the production point at $t = 0$ to the first interaction with medium at time t . Therefore, there is an important finite-size effect for radiation spectrum in a thin medium, and so is the associated energy loss of the leading parton. The finite size effect is important for phenomenological study, because the QGP fireball from nuclear collisions is far from an “infinite” medium.

3.3.3 Numerical solution

To go beyond the above approximation and investigate how different limiting regimes are connected, one has to use a numerical approach. We follow the approach described in [95] to solve the propagator G in the momentum space. Neglecting the thermal mass term, the momentum space representation of the splitting rate is,

$$\frac{dR_{bc}^a(t)}{dx} = \frac{P_{bc}^{a(0)}(x)}{2\pi x(1-x)E} \Re e \int \frac{d\mathbf{p}^2}{(2\pi)^2} \int_0^t d\tau e^{\frac{-i\tau}{\tau_f(p)}} \vec{p} \cdot \vec{\Psi}(\vec{p}, \tau) \quad (3.84)$$

with the time evolution of the vector-valued wave function solved in the interaction picture with the initial condition,

$$\frac{\partial \vec{\Psi}}{\partial \tau} = -e^{\frac{-i\tau}{\tau_f(p)}} \mathcal{C}_3 \left[e^{\frac{i\tau}{\tau_f(p)}} \vec{\psi}(\vec{p}, \tau) \right] \quad (3.85)$$

$$\vec{\Psi}(\vec{p}, \tau = 0) = \mathcal{C}_3 \left[\frac{i\vec{p}}{p^2 + m_{\text{eff}}^2} \right] \quad (3.86)$$

The \mathcal{C}_3 operation involves finite difference and two-dimensional integration over the transverse momentum p . Fortunately the integration over the azimuthal angle of p can be performed analytically at least for the leading order collision kernel with fixed coupling constant. Reparametrize the vector function into a vector part times a rotational invariant function

$\vec{\Psi} = \vec{p}/(p^2 + m_{\text{eff}}^2)^2 \Phi(p^2)$, then the evolution equation for the scalar function Φ is,

$$\frac{\partial \Phi(p^2)}{\partial \tau} = -\alpha_s T \sum_n c_n \int dq^2 \left\{ \frac{\Phi(p^2)}{|p^2 - q^2|} - \frac{\Phi(p^2)}{\sqrt{(p^2 + q^2 + m_n^2)^2 - 4p^2 q^2}} \right\} \quad (3.87)$$

$$\begin{aligned} \Phi(\tau = 0) &= i \sum_n c_n \int dq^2 \left\{ \frac{p^2 + m_{\text{eff}}^2}{|p^2 - q^2|} - \frac{p^2 + m_{\text{eff}}^2}{\sqrt{(p^2 + q^2 + m_n^2)^2 - 4p^2 q^2}} \right. \\ &\quad \left. - \frac{(p^2 + m_{\text{eff}}^2)^2}{2p^2(q^2 + m_{\text{eff}}^2)} \left[\frac{p^2 + q^2}{|p^2 - q^2|} - \frac{p^2 + q^2 + m_n^2}{\sqrt{(p^2 + q^2 + m_n^2)^2 - 4p^2 q^2}} \right] \right\} \end{aligned} \quad (3.88)$$

Here, the summation goes over the different pieces of three-body collision kernel, where the original integration variable \vec{q} has been shifted to $\vec{p} - \vec{q}$, $\vec{p} + x\vec{q}$, and $\vec{p} + (1-x)\vec{q}$ accordingly. The color factors are $c_1 = (C_b + C_c - C_a)/2$, $c_2 = x^2(C_a + C_c - C_b)/2$, $c_3 = (1-x)^2(C_a + C_b - C_c)/2$, and screening masses $m_1^2 = m_D^2$, $m_2^2 = x^2 m_D^2$, $m_3^2 = (1-x)^2 m_D^2$. The azimuthal integration over ϕ_q has been performed analytically, and the resultant operator only involves an integration over q^2 from zero to infinity. One may notice that one of the denominator $|q^2 - p^2|$ can vanish. But as q^2 tends to p^2 , the subtracted term in the second line also approaches the expression in the first line, and therefore leaves the function to be integrated finite. Now, the problem has been reduced to an initial value problem of a 1+1 D first order differential-integral equation, and can be solved quite efficiently using finite difference and numerical quadrature methods.

3.3.4 Mass effect in medium-induced branching

For radiation in the vacuum, the heavy quark mass is a natural regulator for the collinear divergence,

$$\frac{dP}{dx dk_\perp^2} = \frac{\alpha_s P(x) k_\perp^2}{(k_\perp^2 + x^2 M^2)^2} = \frac{\alpha_s P(x)}{k_\perp^2} \left(\frac{\theta^2}{\theta^2 + \theta_M^2} \right)^2 \quad (3.89)$$

Compared to light quark, the radiation off a heavy quark is suppressed within a typical angle $\theta_M = M/E$. This is often referred to as the “dead-cone” (mass) effect [96].

Inside a medium, the situation is more complicated [97–100]. The mass

not only changes the propagator, but also shorten the formation time

$$\tau_f = \frac{2x(1-x)E}{k_\perp^2 + m_{\text{eff}}'^2}, m_{\text{eff}}'^2 = (1-x)m_\infty^2 + x^2M^2 \quad (3.90)$$

These two competing feature together contribution to the mass correction. In principle, the above formula allows for the inclusion of heavy flavor, as long as $M \ll p$ still holds. In the region where $p/M < 1/g$, the radiation process for heavy quark becomes sub-dominant compared to the elastic collisions [101].

3.3.5 Treating multiple emissions

The formula discussed that has been discussed in this section only computes the radiation probability of a single radiation. In reality, the averaged number emissions obtained with this formula can be greater than one, so one has to find a strategy to include multiple emission. There has been two majorly used approaches to resum multiple emissions. The first one is the modified DGLAP evolution approach for the high virtuality partons [102, 103]. The single medium-induced emission probability is added to the vacuum splitting function, and then one applied the DGLAP evolution as in proton-proton collision, but using the so-called modified splitting function. At low virtuality, the parton's in-medium dynamics is more conveniently described as a time evolution. And the rate equation is used to generate multiple emissions in the course of time [90, 104, 105]. The problem that naturally arises is how to interface these two techniques in a realistic events, where an initial highly virtual parton transits to an in-medium transport parton. We shall discuss our tentative solution in the next chapter.

3.4 A modified transport model for the LPM effect

In this section, we shall investigate the approximation to include LPM effect approximately in a particle based Boltzmann transport simulation, termed "a modified Boltzmann transport". Then, we compare the simulation of the "a modified Boltzmann transport" to theoretical calculations introduced in the previous sections for different parton energy, coupling constants, and medium temperatures that are relevant for phenomenology applications. Such a model validation is important as it tells whether the model is a good proxy of the underlying theory and quantifies the theoretical uncertainty

when applying the model to phenomenology study and transport parameter extraction. The approach is designed to work in a large medium and interpolates the deep-LPM region and the Bethe-Heitler region. However, we also check its prediction for finite and expanding medium in the end. The inclusion of running coupling effect and mass effect for the study of heavy-flavor is discussed.

3.4.1 Modifying single particle evolution

To see how to approximate the branching using a modification to the Boltzmann equation, we first go back to the branching probability formula introduced previously [95],

$$\frac{dP_{bc}^a}{dx} = \int_0^\infty dt \frac{g^2 P(x)}{2\pi x(1-x)} \int_t^\infty dt' F(t', t), \quad (3.91)$$

$$F(t', t) = \Re e \int \frac{dp^2}{(2\pi)^2} e^{-it'/\tau_f} \vec{p} \cdot \Psi(\vec{p}, t'). \quad (3.92)$$

We have abbreviate the transition amplitude by the notation $F(t', t)$ for convenience, but always keep in mind this is a quantity that depends on E, ω, g and complete medium properties along the path of the parton, including temperature and fluid velocity profiles $T(t), u^\mu(t)$. The obstacle towards the Boltzmann formulation is the double time integral that signature the quantum transition, which also suggests a fundamental change to the semi-classical approach.

If the time-dependent wave-function is expanded in a series of the collision operator, then this transition amplitude includes the superposition of arbitrary number of multiple-interaction with the medium. Though multiple scatterings of the branching partons also presents in the Boltzmann simulation, the difference is that the Boltzmann multiple-scatterings are independent from the branching processes; therefore, they only broaden the relative transverse momentum *without* changing the branching probability. While from the leading-log approximation, we see that the branching probability should be reduced by a factor $\sim \lambda/\tau_f$. Our modified approach follows this simple observation, and as an overview:

1. Assume an incoherent branching processes is generated at $t = t_0$. Do not treat the daughter partons as independent immediately.
2. Both mother and daughter partons receives elastic broadening from interacting with the medium, which also changes the formation time of the branching.

3. Evolve the branching system until $t - t_0 > \tau_f$. Then, reject this branching process with acceptance probability that is proportional to λ/τ_f , which corrects for the fact that these multiple scatterings should contribute coherently.
4. Branching partons for those accepted processes are treated as independent objects from this point, rejected partons are

Now we shall explain it in detail. Formally, this method can be understood as replacing the transition amplitude $F(t', t)$ by an ensemble (N) of branching systems using the following ansatz,

$$F(t', t) \rightarrow \frac{1}{N} \sum_{i=1}^N \frac{b}{\tau_i(t)} \delta(t - t' - a\tau_i(t)). \quad (3.93)$$

Each copy “ i ” that evolves under the incoherent Boltzmann dynamics will have a certainty probability to have a certain $\tau_i(t)$ at time t . The δ -function expresses that the branching that start at time t' is thought to be formed at time $t + a\tau_f$. The additional factor b/τ_f corrects for that the probability for a branching to happen is different from the incoherent expectation. This ansatz of representing a two-point function using information at t and t' of an ensemble of particles follows the same spirit in the Monte-Carlo solver of the traditional Boltzmann equation, where the distribution function is represented by an ensemble of particles at time t , $n(t, p, x) \approx \frac{1}{N} \sum_i \delta(x - x_i - v_i(t)) \delta(p - p_i)$. This is indeed a crude proxy of the actually two-point function, and its validity has to be examined by comparing its prediction with the theoretical calculations. Finally, a and b are dimensionless factors whose forms shall be determined later and will be tuned to achieve an optimal level of agreement to theoretical calculations.

Plug this simplified ansatz for $F(t, t')$ into the branching probability,

$$\frac{dP_{bc}^a}{dx} = \frac{1}{N} \sum_i \int_0^\infty dt \frac{g^2 P(x)}{2\pi x(1-x)} \frac{b}{\tau_i} \quad (3.94)$$

$$= \frac{1}{N} \sum_i \int_0^\infty dt \frac{g^2 P(x)}{2\pi x(1-x)} \frac{b\tilde{\lambda}}{\tau_i(t = t' + \tau_i)}. \quad (3.95)$$

$$= \frac{1}{N} \sum_i \int_0^\infty dt \frac{dR_{\text{incoh}}}{dx} \frac{b\tilde{\lambda}}{\tau_i(t = t' + \tau_i)}. \quad (3.96)$$

In the second line, we divide and multiplied back an effective mean-free-path $\tilde{\lambda} = m_D^2/\hat{q}_g$. In doing so, the first factor is interpreted as the incoherent

branching rate R_{incoh} , while the second factor is simple the acceptance factor for incoherent branching samples we introduced before. The formation time can be determined self-consistently for each branching copy as it is evolved under the influence of elastic broadening. It is determined at the momentum when

$$t - t' < \tau_f(t). \quad (3.97)$$

This iterative approach for determine τ_f was first developed and implemented by [106]. In the deep-LPM region where the number of rescattering is large, such a procedure reproduce the expected scaling of the average formation time $\langle \tau_f \rangle \propto \sqrt{\omega/\hat{q}}$. This approach also generalizes to medium with a varying temperature profile as the re-scatterings are performed locally as the probe propagate through the medium. In cases where the formation time is short that the acceptance probability is bigger than unity, the acceptance is set to one and the incoherent rate is recovered as the branching with $\tau_f < \tilde{\lambda}$ has entered the Bethe-Heitler regime. Therefore, this approach natural provides an interpolation of the deep-LPM for energetic branching and the Bethe-Heitler regime for soft branching in a large medium.

Now we will determine the form of a and b parameters with guidance from the theory in the deep-LPM region. In the leading-log formula, the average inverse formation time is $\langle \tau_f^{-1} \rangle \sim \sqrt{\hat{q}_3/2x(1-x)E}$. One notice that the effective \hat{q}_3 is different from the \hat{q} of a daughter parton, where we perform momentum broadening. \hat{q}_3 is related to the gluon \hat{q} by the process- and x -dependent factor C_{abc} that has been defined before. For this reason, we chose the a parameter to be this color combination for each branching channel.

$$a \rightarrow a_{abc}(x) = \frac{C_A}{C_{abc}(x)} \quad (3.98)$$

In this way, the formation time for different processes is determined by performing the rescattering broadening of the gluon.

From the previous theory discussion, we know that there is a logarithmic ambiguity in the cut-off scale Q_0 in \hat{q}_3 , and can be determined at the next-to-leading-log level to be the same order as the branching transverse momentum. We need to address what the Q_0 scale is in the Boltzmann simulation and how to improve on top of that. Because the large- Q part of the elastic rescatterings also uses vacuum two-body matrix-elements, the upper bound of the momentum transfer integration is cut-off by the center-of-mass energy \sqrt{s} of each independent collision,

$$s = (p_1 + p_2)^2 = 2E_1 E_2 (1 - \cos(\theta)) \quad (3.99)$$

where p_1 and p_2 are the four momenta of the hard parton and the medium parton. Since at high energy, the cross-section evolves slowly with \sqrt{s} , we can define the average \sqrt{s} by simply averaging p_2 over the thermal distribution,

$$2p_1 \frac{\int p_2^3 e^{-p_2/T} (1 - \cos \theta) dp_2 d\cos \theta}{\int p_2^2 e^{-p_2/T} dp_2 d\cos \theta} = 6ET. \quad (3.100)$$

Therefore, the average Q_0^2 from the independent transport simulation is $6ET$, compared to NLL choice of $\sqrt{\hat{q}\omega}$. The prediction from such simulation would be systematically deviated from theory prediction in a logarithmic manner, varying energy, temperature and coupling constant. To use the correct scale, we define a scale-dependent acceptance probability to correct the naïve choice of $Q_0 \sim \sqrt{6ET}$ with a b parameter,

$$b = 0.75 \sqrt{\frac{\ln(\hat{Q}_1^2)}{\ln(\hat{Q}_0^2)}}. \quad (3.101)$$

with \hat{Q}_1^2 and \hat{Q}_0^2 given by,

$$\hat{Q}_1^2 = 1 + \frac{\sqrt{\omega\hat{q}}}{m_D^2} \approx 1 + \frac{\tau_f}{\lambda} \quad (3.102)$$

$$\hat{Q}_0^2 = 1 + \frac{6ET}{m_D^2} \quad (3.103)$$

The 0.75 is a constant determined when tuning the simulation to theoretical calculations in the next section, and it will be the same throughout the entire work. The origin of this logarithmic ambiguity comes from the perturbative large- q^2 tail the vacuum t -channel matrix-element, based on perturbative argument. However, if one assumes an absence of such a slowly decaying tail in q^2 , such as non-perturbative physics motivated coupling between hard parton and the medium, the logarithmic part in the b -parameter is not necessary.

3.4.2 Implementing mass effect

Heavy quark's large mass $M \gg T$ and unique flavor make it an excellent probe and we would like to apply the aforementioned approach to study heavy flavor as well. Of course, both the theory and the method described should only work in the limit that the parton energy is still large compared to the heavy quark mass. In the region $p \lesssim M/g$ at weak coupling,

the $M/E \ll 1$ breaks down and the elastic energy loss starts to dominate over radiative processes.

Considering that heavy quark introduces a mass correction to the Fermion propagator, the most *naïve* change is to include the mass effect in both the formation time and also the few-body matrix-elements,

$$\tau_f = \frac{2x(1-x)E}{k_\perp^2} \rightarrow \frac{2x(1-x)E}{k_\perp^2 + x^2 M^2} \quad (3.104)$$

and

$$\overline{|M|^2}_{2\leftrightarrow 2}(m=0) \rightarrow \overline{|M|^2}_{2\leftrightarrow 2}(m=M) \quad (3.105)$$

$$\overline{|M|^2}_{2\leftrightarrow 3}(m=0) \rightarrow \overline{|M|^2}_{2\leftrightarrow 3}(m=M) \quad (3.106)$$

For elastic scatterings, this replacement using the massive version of the two-body matrix-element is justified because subsequent elastic collisions are incoherent at weak coupling limit. For inelastic scatterings, again the problem comes from the coherence over multiple scattering centers. At high energy, a heavy quark acquires an average transverse momentum $\hat{q}\tau_f$ larger than the typical transverse momentum of the few body matrix-element $\overline{|M|^2}_{2\leftrightarrow 3}$. As a result, the mass-effect should be less important compared to the scale $\hat{q}\tau_f$ than comparing to the transverse momentum acquired from a single collision center. To solve this problem in the simulation, we choose to use the dead-cone approximation for the radiation off a heavy quark. The $2 \rightarrow 3$ and $1 \rightarrow 2$ branching of the heavy quark is sampled from the massless calculation, while the formation time is determined using the massive formula. The key change is that the acceptance probability is modified by the dead-cone factor,

$$\frac{b\lambda}{\tau_f} \rightarrow \frac{b\lambda}{\tau_f} \left(\frac{k_\perp^2}{k_\perp^2 + x^2 M^2} \right)^2 \quad (3.107)$$

but note that the k_\perp here is the branching transverse momentum after the elastic momentum broadening, and on average $\langle k_\perp^2 \rangle = \langle k_{0,\perp}^2 \rangle + \langle \tau_f \hat{q} \rangle$, where $\langle k_{0,\perp}^2 \rangle$ is the average transverse momentum sampled from the the $2 \rightarrow 3$ matrix-element. One may argue the accuracy of approximating the massive version of the complicated multiple scattering matrix-element using a dead-cone approximation. To evaluate the accuracy of this procedure, we will also compare the radiation spectrum off the heavy quark to the exact solution for heavy quark.

3.4.3 Implementing the running of α_s

There are two places in the transport model where the running of the strong coupling constant might be important: the coupling between the hard patron and the medium, and the coupling constant for the branching vertices. These two processes often happens at different scales.

For the \hat{t} -channel elastic interaction the scale would be the \hat{t} -channel momentum transfer, the typical scale is on the order of the screening mass $|\hat{t}| \sim m_D^2$. Using leading order running of α_s , $n_f = 3$ and $\Lambda = 0.2$ GeV,

$$\alpha_s(Q^2) = \frac{4\pi}{9 \ln(Q^2/\Lambda^2)} \quad (3.108)$$

the coupling constant will blow up with the scale getting close to the non-perturbative scale Λ^2 , and applying leading order perturbative calculation to such regions is problematic. However, in phenomenological application, the temperature of the medium inevitably evolves down to the critical temperate and the scale of the elastic scattering processes is getting too close to Λ^2 . We therefore introduce a minimum scale in the running coupling, proportional to the temperature $Q_{\text{med}} = \mu\pi T$, to regulate the leading order running formula. Of course, regulating α_s to a finite number using such a medium scale does not necessarily improve the accuracy of using the leading order calculation in this temperature range. For example $\alpha_s(2\pi T)$ ranges from 0.28 to 0.45 ($g \sim 1.9 - 2.4$) for temperature decreasing from $T = 0.4$ GeV to T_c , which are extremely large values, considering the next-to-leading-order correction to the probe-medium correction is $O(g)$ ¹.

Unlike the coupling between hard parton and the medium, the scale for the splitting process are much harder than the screening mass. In a static medium, this is because that splitting with a short formation time (compared to the mean-free-path) involves a large transverse momentum $k_\perp^2 > 2x(1-x)E/\lambda \sim m_D\omega/T$, while splitting with longer formation time receives multiple scattering contribution and the average k_\perp^2 scales like $\sqrt{2x(1-x)E\hat{q}} \sim m_D^2\sqrt{\omega/T}$. Therefore for splitting where both the daughter patrons are hard $xE, (1-x)E \gg T$, the running of the splitting vertex coupling is under better control than the probe-medium coupling. For the case of an expanding and fluctuating medium, we shall use a realistic simulation to study the distribution of the actually couplings in the model to access the applicability of the perturbative approach.

¹As a remark, in the final model-to-data comparison, we try to parametrize the non-perturbative contribution by a diffusion processes in our model to prevent the attempt to explain the coupling to sQGP in a pure pertrubative framework.

From [87], the elastic collision couplings are evaluated at \hat{t} -channel momentum transfer q_\perp^2 . This involve both the α_s in the large- q matrix-element ($2 \leftrightarrow 2$, and the elastic matrix-element factorized in $2 \leftrightarrow 3$) as well as the α_s in the soft transport coefficients \hat{q}_S and $\hat{q}_{S,L}$. For the splitting vertex, on the theoretical side it is included by changing the \hat{q}_3 in the NLL formula to its running version [87],

$$\hat{q}_3^{\text{running}} \approx \frac{4\pi}{9} \left(g^2(m_D^2) - g^2(Q_0^2) \right) 1.27 T^3 C_{abc}(x) \quad (3.109)$$

And then evaluate the splitting α_s around an averaged scale (note that k_\perp^2 in the simulation fluctuates a lot),

$$\langle k_\perp^2 \rangle \sim m_D^2 \sqrt{E/T \ln(E/T)} \quad (3.110)$$

For transport simulation, the running of splitting vertex requires a two-step implementation. First, the α_s for the splitting vertex in the few body matrix-element is evaluated at k_\perp^2 . Next, at the end of the elastic broadening for each splitting processes, the acceptance probability is multiplied by a running coupling factor

$$p^{\text{running}} = p \times \frac{\alpha_s(k_{\perp,t_0+\tau_f}^2)}{\alpha_s(k_{\perp,t_0}^2)}. \quad (3.111)$$

Where k_{\perp,t_0}^2 is the transverse momentum when the splitting is generate from the few-body processes, while $k_{\perp,t_0+\tau_f}^2$ is the final transverse momentum including the elastic broadening, and is on average greater than k_{\perp,t_0}^2 .

3.5 Validating the modified transport approach

In this section, we first compare the splitting rate $dR/d\omega$ that comes out of the modified Boltzmann approach simulation to the NLL approximation in the infinite medium limit. Then, we apply the model to a finite and expanding medium, outside of the region where this approach is designed for. Nevertheless, a good qualitative agreement with theoretical calculation of the finite size effect is achieved. In the end, the mass effect implementation is also validated.

3.5.1 In a large and static medium

In practice, to define a Monte-Carlo transport simulation an infinite medium limit and an eikonal limit of parton propagation, an ensemble of parton of

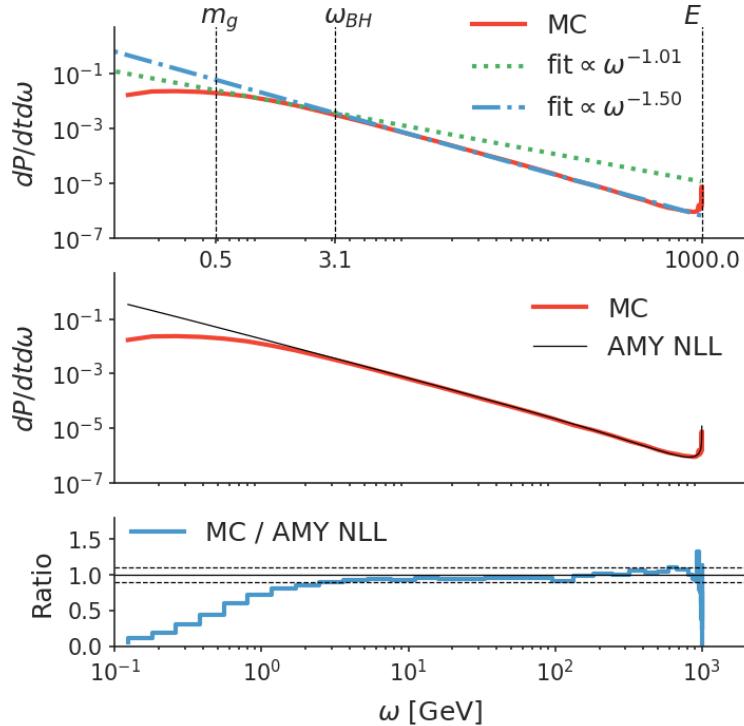


Figure 3.1 The $q \rightarrow q + g$ splitting rate simulated in an infinite box with $T = 0.5$ GeV. The quark energy is $E = 1$ TeV. $\alpha_s = 0.1$. In the top plot, the spectrum $dR/d\omega$ (red line) is fitted to a power function ω^λ in different gluon energy regions. The green dashed line is fitted in the Bethe-Heitler region $\omega < \omega_{BH} \approx 2\pi T$; the blue dash-dotted line is fitted in the LPM region $\omega > \omega_{BH}$. The middle plot compares to the simulation to NLL solution to the AMY equation, and their ratio is shown in the bottom plot

certain species are initialized at a fixed energy E_0 and will be let propagate in the same direction. Each time when a parton scatters elastically or splits, its splitting kinematics are taken down $\omega, k_\perp, t_0, \tau_f$, then the mother parton's energy is reset back to its initial value. For elastic re-scatterings in the implementation of the LPM effect, the parton's energy is re-scaled back to the value before scatterings without changing its direction. The system is evolved for a sufficiently long time t_{\max} , and only branchings that takes place within $[t_{\min}, t_{\max}]$ are analyzed to focus on the infinite time behavior of the simulation.

We start from the $q \rightarrow q + g$ channel. The differential rate $dR/d\omega$ for a 1 TeV quark propagate through a medium of $T = 0.5\text{GeV}$ with coupling constant $\alpha_s = 0.1$ is shown in figure 3.1. The vertical axis is the differential branching rate $dR/d\omega$, and the horizontal axis is the energy of the final state gluon ω . To better understand our result, we have put three “landmark” energy scales in the upper plot, which are the initial parton energy E , an estimate of the Bethe-Heitler energy $\omega_{\text{BH}} \hat{q}_g \lambda_g^2 \sim 2\pi T$, and the screening mass $m_g = m_D/\sqrt{2}$. In the LPM regime $\omega_{\text{BH}} < \omega$, the spectrum falls off as a power law with fitted exponent -1.50 (the blue dash-dotted line), and the in the Bethe-Heitler regime above the screening mass $m_g < \omega < \omega_{\text{BH}}$, the fitted power law exponent is close to -1 (the green dotted line). These exponents are in good agreement with the theoretically expectation that $dR_{\text{BH}}/d\omega \propto \omega^{-1}$ and $dR_{\text{LPM}}/d\omega \propto \omega^{-3/2}$. The screening mass regulates the soft divergence of the spectrum below m_g . One may notice a tiny increase of the spectrum when $\omega \rightarrow E$, this is region where the gluon takes a larger fraction of the initial quark's energy.

In the middle plot, we compare this result from simulation directly to the NLL solution of the AMY equation. As a remark, we have tuned the prefactor in the b -parameter to be 0.75 by comparing to this theory prediction at $\alpha_s = 0.1, E = 1\text{TeV}, T = 0.5\text{GeV}$ for the $q \rightarrow q + g$ channel. For the rest of the comparison with different coupling, parton energy, temperature, and channels, this parameter will **not** be further tuned. The simulation agrees with the NLL solution very well when $\omega \gg \omega_{\text{BH}}$ where the formula is valid. The bottom plot show the ratio between the simulation and the theory, an level of $\pm 10\%$ agreement in the deep-LPM region is achieved in the static case.

Next, we would like to compare the simulation all the three channels in figure 3.2. The setup is the same as the figure 3.1. The red, green and blue lines correspond to the differential branching rate of processes $q \rightarrow q + g^*$, $g \rightarrow g^* + g^*$ and $g \rightarrow q^* + \bar{q}$; the thin back lines are the NLL solution to the

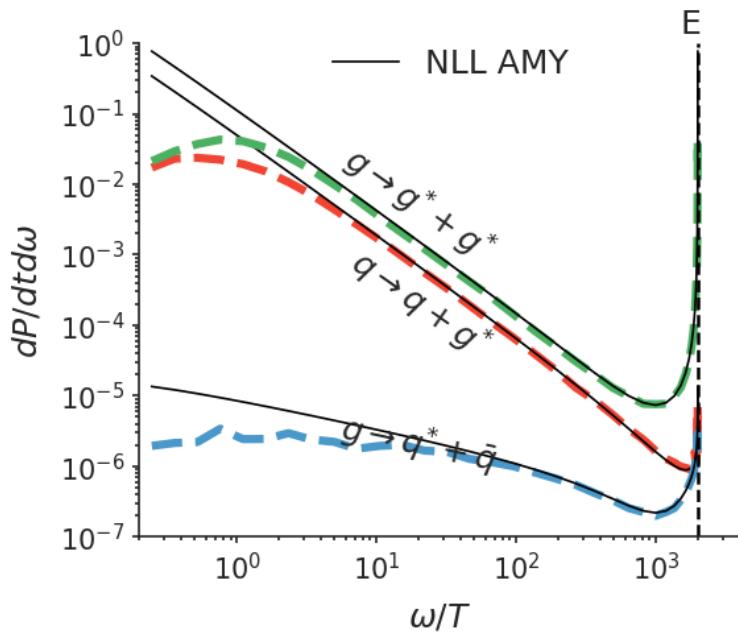


Figure 3.2 The rate of different channels $q \rightarrow q + g^*$, $g \rightarrow g + g^*$, and $g \rightarrow q^* + \bar{q}$ are plotted as functions of the daughter (labeled by "**) parton energy. The mother parton has a energy $E = 1$ TeV. The medium temperature is $T = 0.5$ GeV. $\alpha_s = 0.1$. The simulations (thick dashed lines) are compared to the NLL solutions (thin solid lines).

AMY equation. The “*” sign denotes the final state parton whose energy is ω . For the case two final state gluons, both are taken into account in the simulation as they are identical particles. We have discussed the feature the $q \rightarrow q + g$ in the previous paragraph. The spectrum shape of $g \rightarrow g + g$ process is very similar to the quark splitting channel in the range $\omega \ll E$, with a higher value. The rate is symmetric with respect to $\omega = E/2$ due to its symmetric final states (though it is hard to tell from this double-log plot), so at large ω , the rate goes up again. The spectrum of $g \rightarrow q + \bar{q}$ is also symmetric with respect to $\omega = E/2$. Though its final state consists of two different particle, the splitting function is still symmetric in this case. We see that the simulation achieves a good agreement with the NLL solution in the deep-LPM region $\omega/T > 10$.

Next, we would like validate the simulation with different coupling constant and parton energies. We choose both a relative small coupling $\alpha_s = 0.1(g \approx 1.1)$ and a value closer to the phenomenology coupling $\alpha_s = 0.3(g \approx 1.9)$, and vary the energy from 10 , 10^2 , to 10^3 GeV. The ratios between the simulation and the NLL solutions are shown in figure 3.3, ?? and 3.5. From these systematic comparison. One see that the simulation reproduces the correct scaling in the LPM region, although due to the decreasing of the parton energy, this region also shrinks. The overall performance of the modified Boltzmann transport in describing the inelastic processes in a large medium is good and under control. One remaining problem is that the systematic deviation for the $g \rightarrow q + \bar{q}$ channel is bigger than the other two channels, as we did not include the backward region in its $2 \rightarrow 3$ matrix-elements.

Finally, we validate the running coupling calculation in Fig. 3.6 using the $g \rightarrow g + g$ channel. The theory curves (black lines) are obtained combining Eq. 3.79 and Eq. 3.109. Different line styles correspond to the variation of the Q_0 value around an initial guess $m_D(E/T \ln(E/T))^{1/4}$ by a factor of 2 above and below. For this 1 TeV parton, the scale Q_0 is actually very large and the running of α_s is rather slow, which explains the theory curve is not very sensitive to a factor of 4 change in Q_0 . The simulation was performed using the running coupling prescription described in Section ???. The overall shape of the spectrum in the deep LPM region is again well described by the modified Boltzmann simulation.

3.5.2 Branching in a finite / expanding medium

We have made clear before that this approach is designed for interpolating the Bethe-Heitler region and the deep-LPM region in a large medium, and from the validation in the previous section, it indeed works very well.

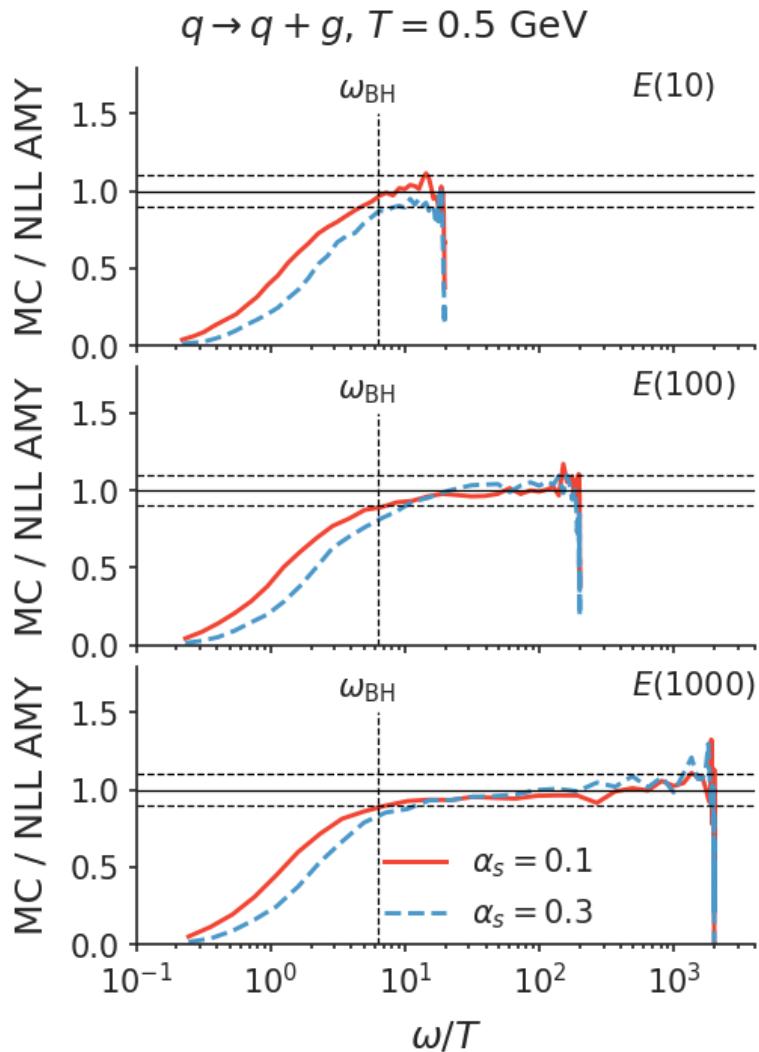


Figure 3.3 Ratios of splitting rate dR/ω between the modified Boltzmann simulation and the NLL solution for $q \rightarrow q + g$ splitting. The quark energies are E is 10, 100, and 1000 GeV from top to the bottom plot. And two coupling constants are used: $\alpha_s = 0.1$ (red solid lines) and $\alpha_s = 0.3$ (blue dashed lines). ω stands for the gluon energy. The horizontal dashed lines denote $\pm 10\%$ deviation from unity.

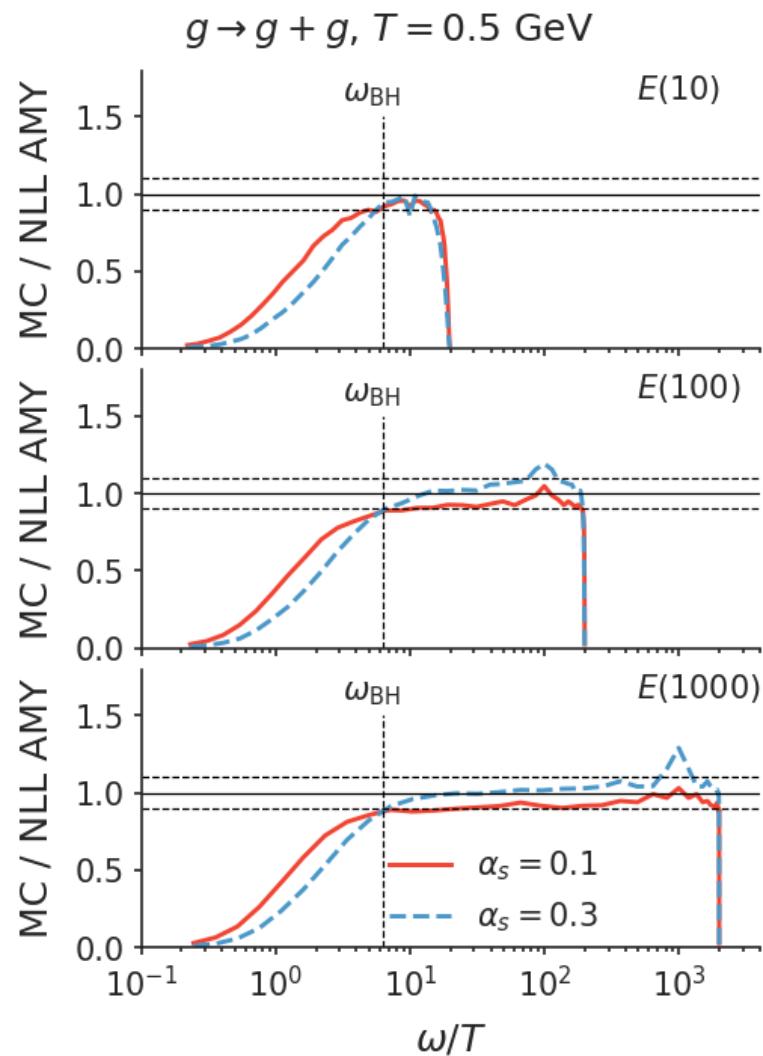


Figure 3.4 The same as figure 3.3, but $g \rightarrow g + g$.

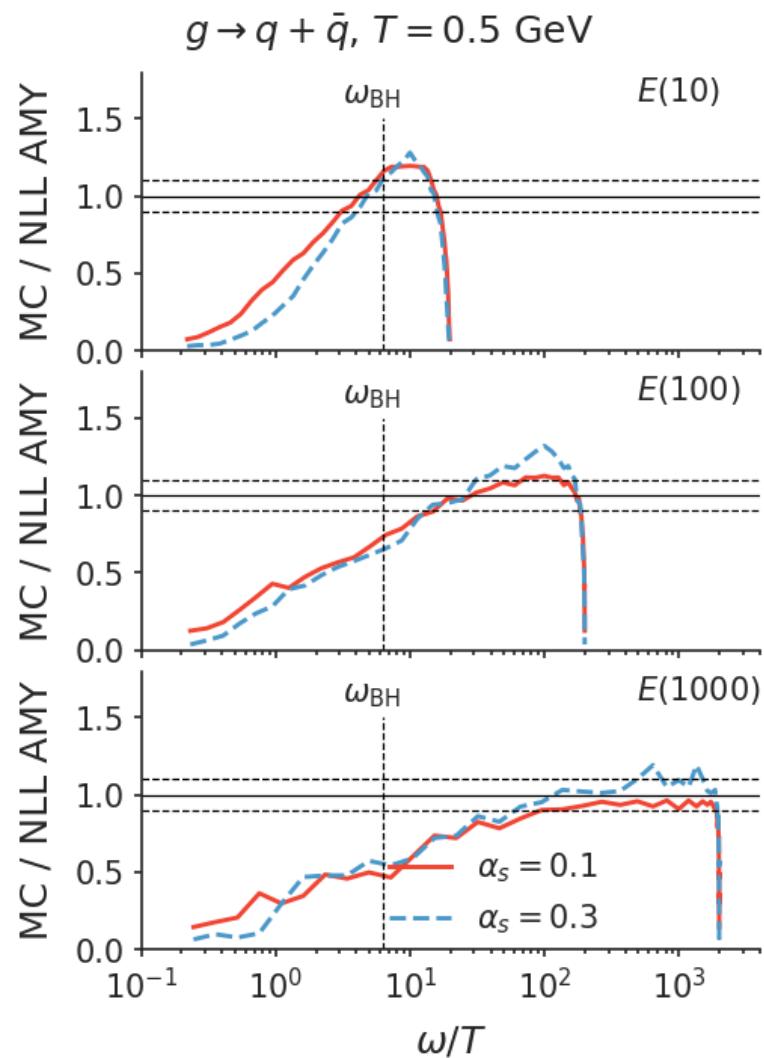


Figure 3.5 The same as figure 3.3, but $g \rightarrow q + \bar{q}$.

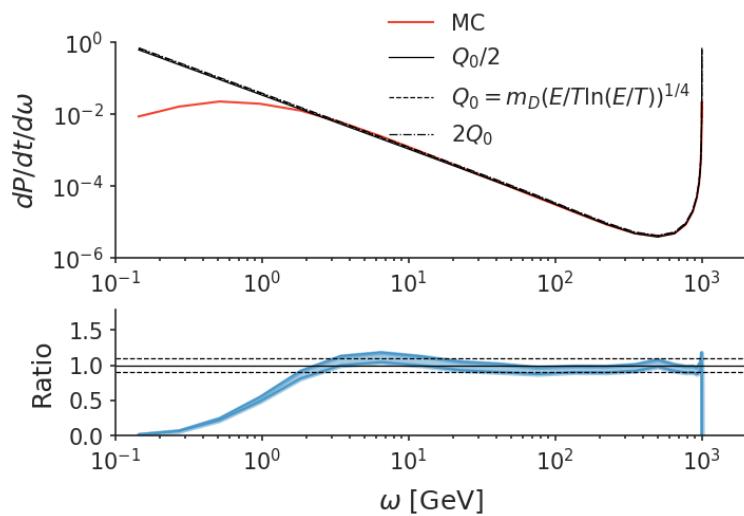


Figure 3.6 Comparing the simulation with running coupling constant the NLL solution with running α_s prescription. The scale Q in the emission vertex and in the theoretical formula for the effective transport parameter \hat{q}_3 (equation 3.109) is chosen to be 1/2, 1 and 2 times of the scale $\sqrt{\langle k_\perp^2 \rangle}$ in equation 3.110. The ratio is shown in the bottom plot.

However, the medium created in heavy-ion collisions were never in the large and static limit, its finite time and spatial extend, local hot spots fluctuations and the fast radial expansion can all make significant impact on the hard parton propagation. Therefore, we need to investigate how our approach would behave in a few more complex scenarios: a finite medium and an expanding medium, before applying such a model to phenomenological usage.

A semi-infinite medium Consider the semi-infinite medium with the static temperature profile,

$$T = \begin{cases} 0, & z < 0 \\ T_0, & z > 0 \end{cases} \quad (3.112)$$

and hard partons are created at $z = 0$ and propagate into the medium. Deep inside the medium, the medium induced radiation should be getting asymptotically close to the calculation in an infinite medium. However, at the boundary, there is a complicated interference between medium scatterings centers and the hard production vertex. For a thin medium where the path length is short compared to the formation time, these interference terms can be worked out in the “opacity (L/λ) expansion”, or by analyzing the propagator in the path-integral formalism with the semi-infinite temperature profile. This boundary effect results in a path length dependence of the medium induced branching rate that starts from zero at $t = 0$ and gradually approach the asymptotic value in a large medium. The resulting parton energy loss rate is significantly reduced due to this effect, and scales quadratic with the path length $\Delta E \propto L^2$ near the boundary (at larger times, it transits to $\Delta E \propto L$). This feature can have significant phenomenology impact in understanding the nuclear modification factor and the azimuthal anisotropy of the leading particles, heavy flavors and jets.

It is true that our approach is designed for a large medium, but it also displays certain finite size effect. Of course, it is can not reach an quantitative level of agreement with the theory at $L \lesssim \tau_f$ since the interference pattern is not implemented. The cause of the finite size effect in our approach can be understood as following. Remember that the branchings in the modified transport approach takes a finite amount of time, and those branching that becomes independent at time t are actually initiated by a $2 \rightarrow 3$ processes at from a wide range of scattering centers in the past $t' = t - \tau_f$. Therefore, if the medium is semi-infinite, and there were no scattering centers before $t' = t - \tau_f < 0$, then the medium-induced contribution to the branchings at time t will be reduced. This reduction gets weaker and weaker when the

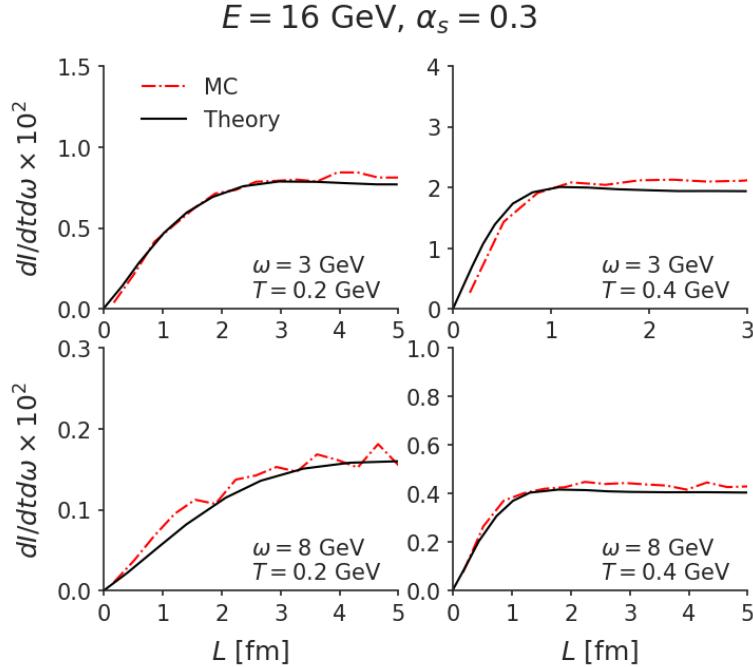


Figure 3.7 The path-length dependence of the simulated $q \rightarrow q + g$ emission rate $dR/d\omega$ compared to the direction calculation of formula 3.91 from [95]. $\alpha_s = 0.3$. The quark energy is 16 GeV. The left and right columns have medium temperature $T = 0.2$ and 0.4 GeV respectively. The top and bottom rows show the differential rate at $\omega = 3$ and 8 GeV.

condition $t - \tau_f > 0$ can be satisfied by more and more induced branchings and eventually, when $t \gg \langle \tau_f \rangle$, this boundary effect dies off in the simulation. We would like to check if this simulation boundary effect qualitatively mimic the interference physics that happens near the boundary.

In Figure 3.10, the differential rate obtained from simulation is compared to the numerical solution of the full leading order calculation inside a finite medium. The horizontal axis is the time of travel by the hard parton (path length divided by the speed of light), and each subplot shows how the branching rate changes as a function of time with different medium temperatures ($T = 0.2$ GeV on the left, $T = 0.5$ GeV on the right) and at different branching parton energy ($\omega = 3$ GeV at the top, $\omega = 8$ GeV at the bottom). The theory curves are taken from the references [95] for a 16 GeV parton with coupling constant $\alpha_s = 0.3$, and the red lines are our simulation. The theory curve first increases linearly and then turn over to a constant value

in the large medium limit for $t \gg \sqrt{2x(1-x)E/\hat{q}_3}$. The simulation, as expected, reproduces the large time limit of the rate. Moreover, we find that the current implementation also predicts the qualitative “turn over” of the spectra at finite path length. The original paper only publish this calculation for a 16 GeV quark. To validate if this qualitative agreement also holds at higher parton energies, we implement the numerical approach [95] and compute the theoretical curves for $E = 100$ GeV partons. The comparison of simulation and numerical solutions are shown in figure 3.8 and again, we found a qualitative agreement with the theoretical finite size effect.

An expanding medium Fast radial expansion is another important feature of the created quark-gluon plasma. It causes the temperature at the medium rapidity to decrease drastically in the early stages of the expansion and introduces another time scale in which the medium temperature changes notably. Assume a simplified power-law changing temperature profile

$$T(\tau; \nu)^3 = T_0^3 \left(\frac{\tau_0}{\tau} \right)^{2-1/\nu}. \quad (3.113)$$

The ν parameter controls the rate of expansion. $\nu = 1/2$ is the static medium limit, and $\nu = 1$ is the Bjorken flow. We can define the following medium expansion time, over which the transport parameter changes significantly,

$$\tau_{\text{ex}} = \left(\frac{d \ln(T^3)}{d\tau} \right)^{-1} = \frac{\tau}{2 - 1/\nu}. \quad (3.114)$$

The larger the ν parameter is, the smaller the expansion time scale. With $\tau_0 \sim 1 \text{ fm}/c$, the expanding time scale can be short enough that energetic branchings already probes the changing temperature profiles within its formation time $\tau_f > \tau_{\text{ex}}$. One consequence of this fast changing of temperature is that, for these branchings $\tau_f > \tau_{\text{ex}}$, the transition probability over a finite amount of time can not be well approximated by integrating rates that are calculated in an infinite box defined by the local temperatures,

$$\frac{dP(t_1, t_2)}{d\omega} \neq \int_{t_1}^{t_2} \frac{dR_\infty(T(t))}{d\omega} dt, \quad (3.115)$$

where is the rate obtained by solving the branching rate in the infinite medium setup. This approach is employed in transport models like MAR-TINI and TEQUILIA [66, 104, 105]. Our approach takes into account the changing of the medium temperature (and also flow velocity). This is because the rescattering procedure that determines amount of suppression is

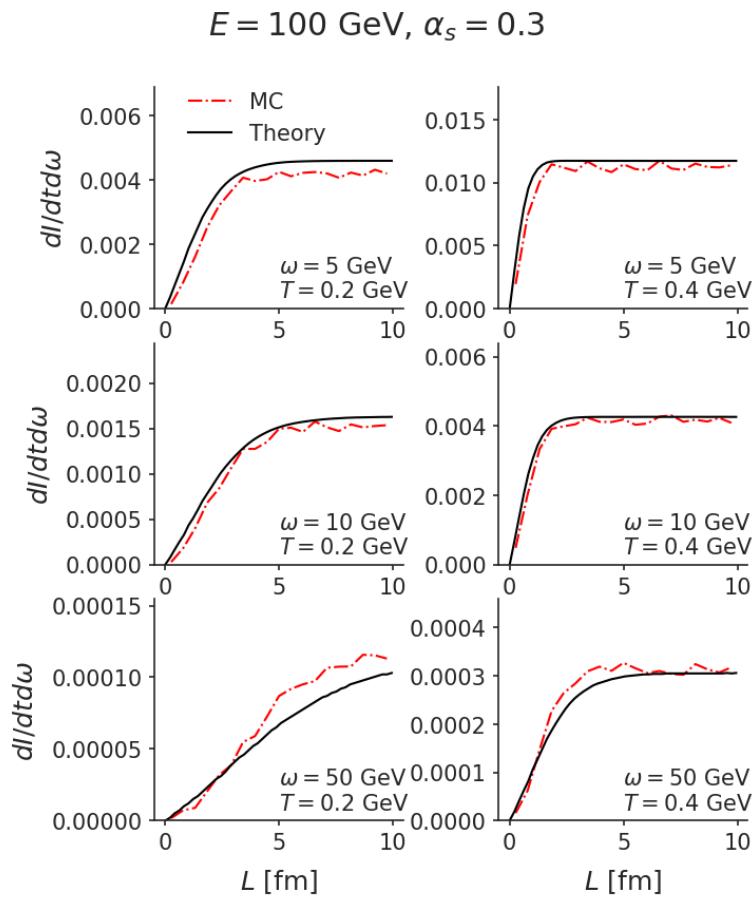


Figure 3.8 The same as figure 3.8, but the initial quark energy is 100 GeV, and is plotted for gluon at 5 (top), 10 (middle) and 50 (bottom) GeV.

performed along the trajectory of the hard partons and therefore naturally includes the effect of the cooling of the medium. The typical formation time determined by the rescattering procedure is also changed by the expansion. Recall that in a static medium the dimensionless combination that enters the leading-log formula is the $t/\tau_f \sim t\sqrt{\omega/\hat{q}}$, but with a \hat{q} that is decreasing with temperature. The self-consistent determination of the formation time requires the following relation to hold on average,

$$t_2 - t_1 = \frac{2x(1-x)E}{k_\perp^2(t_1) + \int_{t_0}^t \hat{q}(\tau)d\tau}, \quad (3.116)$$

$$\hat{q}(\tau) = \hat{q}(\tau_0) \left(\frac{\tau_0}{\tau} \right)^{2-1/\nu} \quad (3.117)$$

Neglecting the initial transverse momentum at $t = t_1$, we have the characteristic time scale $\Delta t = t_2 - t_1$ of this procedure in the expanding medium temperature profile as

$$1 = \sqrt{\frac{\hat{q}(t_0)}{2x(1-x)E}} \tau_0 \sqrt{\frac{\nu-1}{\nu}} \left(\frac{\Delta t}{\tau_0} \right)^{1/2\nu} \quad (3.118)$$

To make comparison to theoretical calculations to see if the simulation procedure also gives a reasonable description in an expanding medium, we make use of a result obtained in the BDMPS framework [81, 85]. Using the power-law decreasing temperature profile, the obtained branching probability is,

$$\frac{dP}{d\omega} = \frac{\alpha_s}{2\pi E} P_{q \rightarrow qg}(x) \Re e \int_{\tau_0}^{\tau_0+L} \frac{dt_f}{t_f} \int_{\tau_0}^{t_f} \frac{dt_i}{t_i} \frac{1}{\nu^2} [I_{\nu-1}(z_i)K_{\nu-1}(z_f) - I_{\nu-1}(z_f)K_{\nu-1}(z_i)]^{-2} \Big|_{\omega=x E}^{\omega=\infty}, \quad (3.119)$$

$$z_{i,f} = 2i\nu \sqrt{\frac{\hat{q}_g(1-x+C_F/C_A x^2)}{2(1-x)\omega}} \tau_0 \left(\frac{t_{i,f}}{\tau_0} \right)^{1/2\nu} \quad (3.120)$$

for the $q \rightarrow q+g$ splitting. This result goes back to the static BDMPS result [81] when $\nu = 1/2$. One potential problem of comparing the formula to our simulation is that this BDMPS calculation works in the multiple-soft limit (leading log). Therefore, we used only the diffusion-induced radiation in the simulation and turned off the large- Q $2 \rightarrow 3$ scattering part. Also as mentioned before, in the absent of the perturbative tail in the collision kernel, $b = 0.75$ is used without the logarithmic correcting factor in equation 3.101. In addition, we will not try to make a direct comparison of the spectra

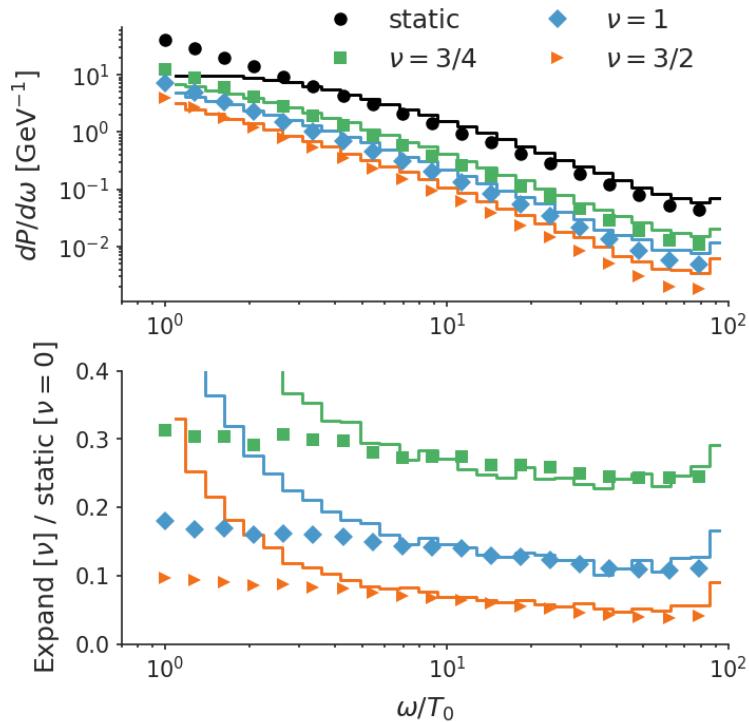


Figure 3.9 Top plot: the simulated spectrum (diffusion plus diffusion-induced radiation only) using the parametric medium with expansion parameters $\nu = 0$ (static, black), $3/4$ (green), 1 (Bjorken, blue), and $3/2$ (orange). The analytic results are shown in symbols and simulations in lines. $\alpha_s = 0.3$. The expansion starts at $\tau_0 = 0.2 \text{ fm}/c$ with an initial temperature $T_0 = 1 \text{ GeV}$. Bottom plot: the ratios between calculation (simulation) in an expanding medium to that in the static medium.

(left of figure 3.9), but focusing more on the ratio between the expanding calculation/simulation over the static calculation/simulation instead. This ratio reflects the change of the shape of the spectra due to the dropping of temperature.

The simulation uses a medium with initial temperature $T_0 = 1$ GeV at $\tau_0 = 0.2$ fm/ c and lasts until $\tau = 20$ fm/ c using four different expansion rate $\nu = 1/2, 3/4, 1, 3/2$. These choice of numbers corresponds to a static medium, a slowly expanding medium, the Bjorken flow, and a faster-than-Bjorken expansion. We found that when $\omega \gg T_0$, the degree of change in the radiation spectra is well reproduced by the modified transport simulations.

3.5.3 Heavy quark and thermalization test

Finally, we check the model performance for heavy quarks. For short, to implement mass effect to the modified transport approach for inelastic scatterings, we use massive kinematics for the heavy quarks, include the mass term in the formation time, and implement the dead cone approximation after the transverse momentum is broadened by elastic collision. The theory curves are obtained by solving the exact equation with a effective mass term,

$$m_{\text{eff}}^2 = (1 - x)m_g^2 + x^2 M^2 \quad (3.121)$$

which includes both the thermal mass of the gluon and the current mass of the heavy quark. We present the comparison between the simulation and the theory in terms of the ratio between the differential branching rate of the heavy quark (charm mass at 1.3 GeV, bottom mass at 4.2 GeV) and the light quark. In figure ?? for the bottom quark case, the horizontal axis is the path-length, and the vertical axis is the ratio. Different rows take different radiated gluon energies, and different columns has medium temperatures at 0.2 GeV (left) and at 0.4 GeV (right) respectively. The initial bottom quark energy is 100 GeV and the coupling is $\alpha_s = 0.3$. We see that the dead-cone approximation better agrees with the theory calculation at larger x and larger path-length. Deviations observed at small path length is understand as the limitation of our implementation to the large medium, and should be better treated by the opacity expansion. The deviation at small x is interesting, particularly, the theory almost predicts an identical heavy quark radiation spectra as the light quark. This absent of dead cone at small- x is already observed in early works of heavy quark energy loss study in both the GLV framework and the BDMPS framework. This means

$$E = 100 \text{ GeV}, \alpha_s = 0.3$$

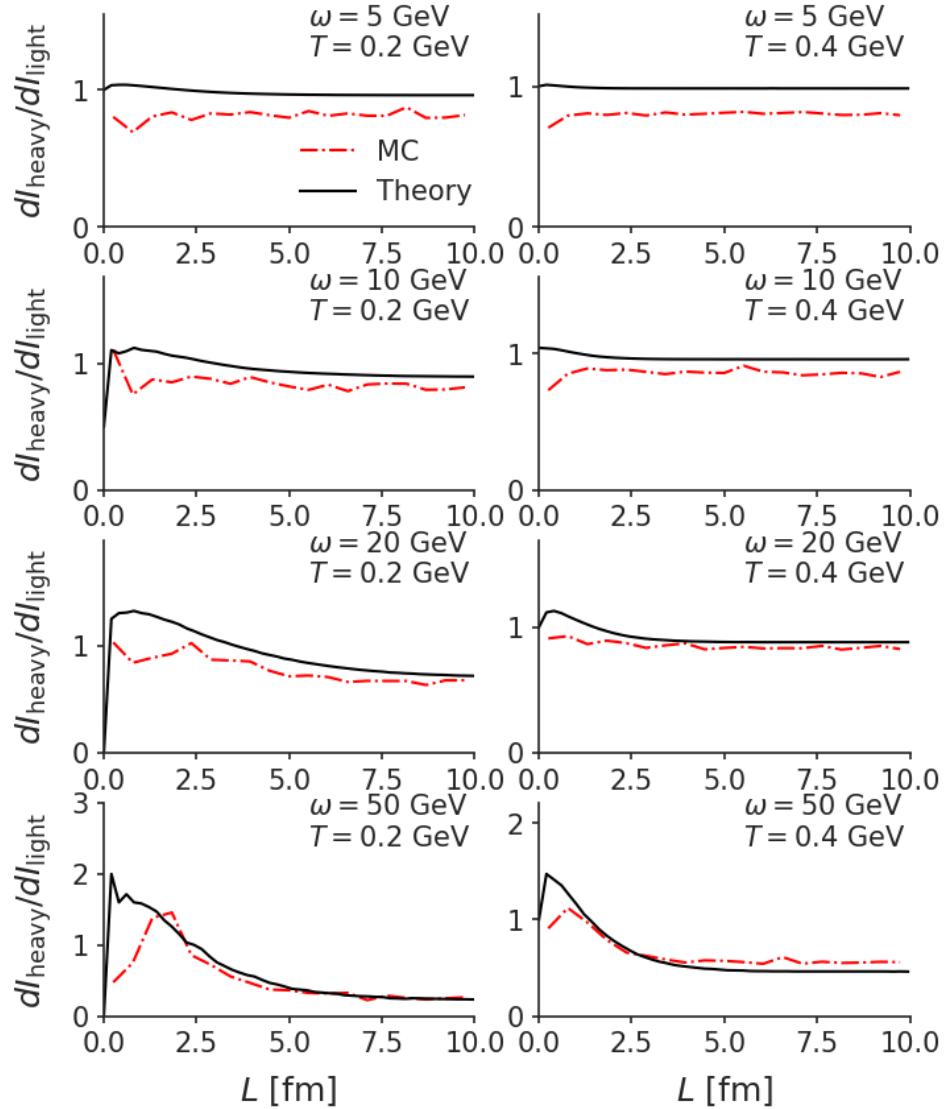


Figure 3.10 The mass dependence of the radiation spectrum $q \rightarrow q+g$, presented as the ratio of bottom $dR/d\omega$ over the light quark $dR/d\omega$, as functions of path length. The left and right columns use temperatures 0.2 and 0.4 GeV. Different rows (from top to bottom) plot cases for gluon energy $\omega = 5, 10, 20, 50$ (GeV).

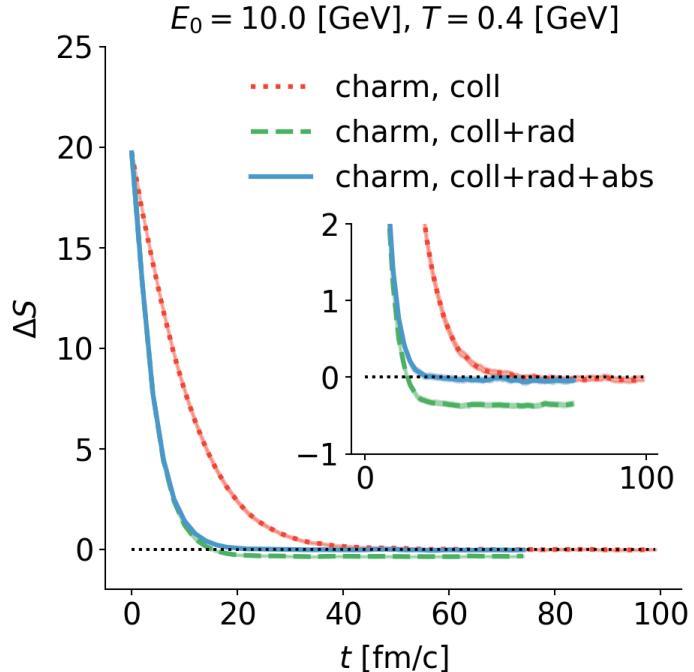


Figure 3.11 Approaching to thermal equilibrium of heavy flavor is quantified as the change of ΔS (defined in equation 3.123) as function of time.. The red dotted lines includes elastic processes only. The green dashed line further includes $2 \rightarrow 3$ and $1 \rightarrow 2$ processes. The blue solid lines turn on the detailed balance processes $3 \rightarrow 2$ and $2 \rightarrow 1$.

that the treatment of the mass effect is not as simple as the dead-cone approximation and should be improved in the future.

Thermalization of heavy quark Heavy quark's large mass made it takes longer time to thermalize and the low- p_T end of the heavy quark production in the heavy-ion collision can carry the information non-equilibrium dynamics. To extract the degrees of thermalization, one has to make sure the correct thermalized limited is achieved in the transport model, given enough time of evolution. This is trivial for large-angle elastic scatterings and diffusion processes as long as the correct Einstein relation is imposed. The $n \rightarrow n + 1$ body radiative process is approximated by a initial $2 \rightarrow 3$ or $1 \rightarrow 2$ process and a sequence of elastic interactions; therefore, in principle

the $n + 1 \rightarrow n$ absorption processes need to be treated on the same footing to restore the detailed-balance in the modified-Boltzmann equation. This can be done but is over complicated. Here we argue that close to a few times of temperature, the LPM effect is not that strong that an incoherent implementation of the absorption is enough to study the bulk of particles close to thermal distribution.

We define a quantity ΔS to measure the approaching of thermal distribution $f_0 = e^{-E/T}$ of an ensemble of heavy quarks,

$$\Delta S = -\langle \ln f_0 \rangle - S_0 \quad (3.122)$$

$$= -\frac{1}{N} \sum_i \ln f_0(E_i) - \frac{\int dp^3 f_0 \ln(f_0)}{\int dp^3 f_0} \quad (3.123)$$

Where the first term is the ensemble average of the function $-\ln f_0$, and the subtracted term is proportional to the entropy of distribution f_0 . Note that the quantity is zero if the ensemble thermalize. If the system is approaching thermal distribution with an effective temperature such that $f = e^{-E/T'}$, then ΔS is

$$\Delta S = \frac{\int dp^3 E / T e^{-E/T'}}{\int dp^3 e^{-E/T'}} - S_0 = \frac{T' - T}{T} \quad (3.124)$$

which is a measure of the deviation of the effective temperature from the thermal bath temperature.

Using this definition, we plotted ΔS as a function of time for 1000 heavy quarks that are initialized at 10 GeV. The temperature of the thermal bath is 0.5 GeV and we used a fixed $\alpha_s = 0.3$. Under the influences of diffusion (red) and diffusion plus large-angle elastic collisions (green), ΔS decreases from a large value until fluctuating around zero after 25 fm/c (red) and 15 fm/c (green). Now, adding the radiative processes (blue), the ΔS reaches a value below zero, which is the false equilibrium. Only after the balancing processes of parton absorption are also included (orange), the correct thermal equilibrium limit is restored. We also found that the absorption process only sets in when the ensemble is close enough to the thermal distribution, as the blue line and the orange line are almost overlapped until ΔS dropped to 0.3. This is because the absorbed gluon follows the thermal distribution in the medium while phase-space for a high energy parton $E \gg T$ to absorb a low energy gluon is very limited $x < T/E$, compared to radiation processes where the value of x is not restricted by the Boltzmann factor $e^{-xE/T}$.

3.6 Comments on two other inelastic process implementations

I find it beneficial to discuss two other inelastic processes implementations for reader's references. They are termed as the "coherence factor" approach and the "blocking radiation" approach. I had used the previous approach in my earlier studies [75], but it is the problems I encountered in this method that later motivates the development of the "modified Boltzmann transport" method. I shall show in this section that in the deep-LPM region, the "coherence factor" approach still qualitatively agrees with the power counting of the LPM suppression λ_{el}/τ_f , though it only includes the effect of one medium scattering centers and the method can be logarithmic dependent on the infrared cut-off. The "blocking radiation" approach, however, does not reproduce the power counting of the LPM suppression. These two approach, together with the "modified Boltzmann" approach will be compared later using the "energy loss" of a fixed energy quark. First, we introduce these two other approaches.

3.6.1 The coherence factor approach

This approach is first implemented in the improved Langevin equation [107], using the single medium-induced radiation probability from the higher-twist calculation [108, 109] and a prescription for multiple emissions. The higher-twist formula of medium-induced radiation is derived for a high virtual parton, including the interference of the hard production vertex and one medium scattering center. The single radiation rate reads,

$$\frac{dN_g}{dx dk_\perp^2 dt} = \frac{\alpha_s P(x) \hat{q}_g}{\pi k_\perp^4} 2 \left(1 - \cos \frac{t - t_0}{\tau_f} \right), \quad \tau_f = \frac{2x(1-x)E}{k_\perp^2} \quad (3.125)$$

Here the radiation rate is a time-dependent (t) one due to the interference with the hard production at time t_i . Note that the interference factor cancels the collinear divergence. The only divergence comes from soft emission $x \rightarrow 0$. This divergence is not a problem for computing more physical quantities such as the energy loss, as it will be balanced by the gluon absorption processes. However, in order to apply rate formulation, an infrared cut-off $x > x_c$ has to be introduced.

The advantage is that if there is only one radiation, then sampling the time dependent rate indeed reproduces the High-Twist calculation. However, the ambiguity rises from the way it handles multiple emissions. For

example, one can compute the average number of emission by integrating this formula along the trajectory of the hard parton through and then samples the fluctuating number of emission with a Poisson distribution. But of course, this would assume the parton energy is not significantly changed during the process, and it is not clear how the presence of more than one scattering center would change this picture. Here we would like to discuss another method in dealing with multiple emission using the high twist formula in a time evolution manner [107]. The algorithm goes as follows:

1. Choose an infrared cut-off for the gluon energy $x_c \propto T/E$, and a small enough time step Δt , so that the average number of emission is much smaller than 1 to suppress multiple emission within Δt ,

$$\langle N_g \rangle = \Delta t \int_{x_c}^1 dx \int dk_\perp^2 \frac{dN_g(t - t_0)}{dx dk_\perp^2 dt} \ll 1. \quad (3.126)$$

2. Sample N according to a Poisson distribution with $\langle N_g \rangle$. For $\langle N_g \rangle \ll 1$, it is sufficient to sample the two leading cases of $N = 0, 1$, as the probability to have more than 1 emission is negligible ($P_{N>2} = 1 - e^{-\langle N_g \rangle} - e^{-\langle N_g \rangle}/\langle N_g \rangle = O(\langle N_g \rangle^2) \ll P_1 \ll P_0$).
3. If $N = 0$ then propagate the parton to the $t + \Delta t$. If $N = 1$, then sample the emission gluon's x , and \vec{k}_\perp by the differential rate. *Meanwhile, t_0 is set to t* , so that the next emission's probability will accumulated from zero again.
4. Proceed for the next time step.

We found that the key step here is resetting the clock $t_0 = t$ for the parton after every emission. As a result, from the second emission, the time difference that appears in the interference factor $t - t_0$ are the one measuring between two medium scattering centers. Therefore, we will not interpret this procedure as the high-twist rate (interference between initial hard vertex and one medium collision center) starting from the second emission; instead we understand it as an ansatz, from the second emission, to treat medium-induced emission in a large medium, as it do not require any information to the production vertex.

Considering it only includes one medium scattering center in the trigger the radiation, one wonders if this approach reproduces any in-medium radiation features predicted by the theory. It is not immediately clear that what this iterative procedure predicts expect through simulations. But if one pondering on the meaning of the “clock resetting” step, then the typical

$\Delta = t - t_0$ between two emissions are a time scale within which the emission probability reaches order one,

$$1 \sim \int_{t_0}^t dt \int_{x_c}^1 dx \int dk_\perp^2 \frac{dN_g(t - t_0)}{dx dk_\perp^2 dt}. \quad (3.127)$$

With this key observation, after a few step of algebra, we are able to learn the qualitative feature of this approach. Taking the soft approximation $P(x) \sim 2/x$, $\tau_f \sim 2xE/k_\perp^2$, and perform the time integral first, then the k_\perp integral with limits from 0 to xE .

$$1 \sim 4\alpha_s \hat{q} \Delta t \int_{x_c}^1 \frac{dx}{x} \int \frac{dk_\perp^2}{k_\perp^4} \left(1 - \frac{\sin(\Delta t/\tau_f)}{\Delta t/\tau_f} \right) \quad (3.128)$$

$$= \alpha_s \hat{q}_g \Delta t^3 \int_{\frac{\Delta t E x_c}{2}}^{\frac{\Delta t E}{2}} \frac{du}{u^2} \frac{u^2 \text{Si}(u) - 2u + \sin(u) + u \cos(u)}{u^2} \quad (3.129)$$

$$= \frac{\alpha_s \hat{q}_g \Delta t^3}{3u^3} \left(u^3 \text{Ci}(u) - 3u^2 \text{Si}(u) - u^2 \sin(u) + 3u - \sin(u) - 2u \cos(u) \right) \Big|_{\frac{\Delta t E x_c}{2}}^{\frac{\Delta t E}{2}} \quad (3.130)$$

This final integral of x (reparametrize by $u = xE\Delta t/2$) would have been logarithmic divergent if we had not cut it at x_c at the lower bound. The result has the following expansion at small u : $\frac{1}{18}(6\ln(u) + 6\gamma_E - 17)$ and decay to 0 at infinite therefore a good proxy is to use the small- u expansion but cut-off the upper bound of u at its zero, and finally

$$1 \sim \frac{\alpha_s \hat{q} \Delta t^3}{3} \ln \frac{2}{x_c E \Delta t} \propto (g^2 T \Delta t)^3 \ln \frac{2}{x_c E \Delta t} \quad (3.131)$$

Now, it is clear that this procedure of implementing multiple emission inside the medium resets the clock in the interference factor every $1/g^2 T$ up to certain logarithm dependence on the infrared cut-off, which is the order of the elastic collision mean-free-path. Put this estimated Δt back into the interference factor $2(1 - \cos(\Delta t/\tau_f))$, one indeed find that the radiation spectrum will be strongly suppressed if the formation time is much greater than $\Delta t \sim \lambda_{el}$.

This suppression certainly mimic some property of the in-medium LPM effect, but is introduced by a very different mechanism. Remember that the LPM effect is the suppression of single particle emission rate through multiple collision with the medium, without any information about how subsequent emissions are correlated. While the interference factor approach

mimic the effect of the LPM suppression through correlation between subsequent emissions. This will introduce several problems:

1. The correlation between subsequent emissions is in fact physics beyond leading order and requires new type of diagrams to be computed.
2. As we have seen, this procedure is affected by the choice of the infrared cut-off. Though its dependence is very weak, it is still a dependence that we try to avoid.

3.6.2 The “blocking radiation” approach

This is another approach we found in the literature [110]. I would like to show that this approach is more problematic than the previous one, because it suppresses radiation with $\tau_f > \lambda_{inel}^{incoh}$ but not $\tau_f > \lambda_{el}$.

In this approach, the splitting is also first generated through an incoherent processes at time t_0 , and then the self-consistently determination the formation time by elastic broadening. But its LPM suppression is introduced by requiring no other radiation is allowed from this radiator within the time from t_0 to $t_0 + \tau_f$. This clearly introduces a correlation between subsequent emission, while the LPM effect concerns only the one particle emission rate. While in our approach, the suppression is implemented by accepting the process with probability $\sim \lambda_{el}/\tau_f$, and more importantly, other emissions are unaffected by the current “imaginary splitting” as most of them would be rejected without causing any physical effect.

A closer investigation reveals bigger problem. Moreover, this “blocking radiation” approach effectively reduces every τ_f/λ_{inel} incoherent emission to one, resulting only an overall reduction in the radiation spectrum without changing its shape. And the suppression factor λ_{inel}/τ_f is different from the expected one, this is in fact an order of α_s wrong as the mean-free-path of the incoherent radiation rate contains one more power of α_s than λ_{el} .

3.6.3 Energy loss comparison among the three approaches

In Figure 3.12, we show the calculation of energy loss per unit path length dE/dx of a quark in an “infinitely large” medium. Technically, dE/dx is measured after an evolution time long enough ($L \gg L_c$) that finite size effects have faded away. The results presented are normalized by $1/(\alpha_s^2 \sqrt{ET^3})$ in anticipation of the scaling $dE/dx \propto \alpha_s^2 \sqrt{ET^3}$. For each column, we double the value of α_s and for each row, the temperature is increased by 0.2 GeV.

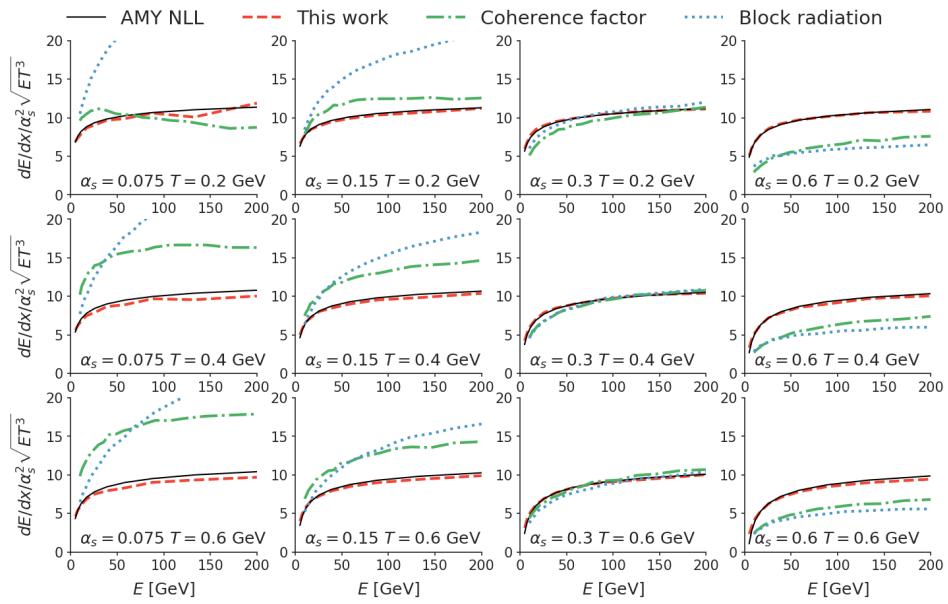


Figure 3.12 Energy loss per unit path length dE/dx as a function of energy E , temperature T and coupling constant α_s . Each column corresponds to a value of the coupling constant $\alpha_s = 0.075, 0.15, 0.3$, and 0.6 (from left to right). Each row corresponds to a temperature of $T = 0.2, 0.4$, and 0.6 GeV (from top to bottom). dE/dx is divided by the expected scaling $\alpha_s^2 \sqrt{ET^3}$. The MC implementations in this work (red dashed lines) is compared to the “coherence factor” approach (green dash-dotted lines) and the “block radiation” approach (blue dotted lines). The analytic results are denoted as black solid lines.

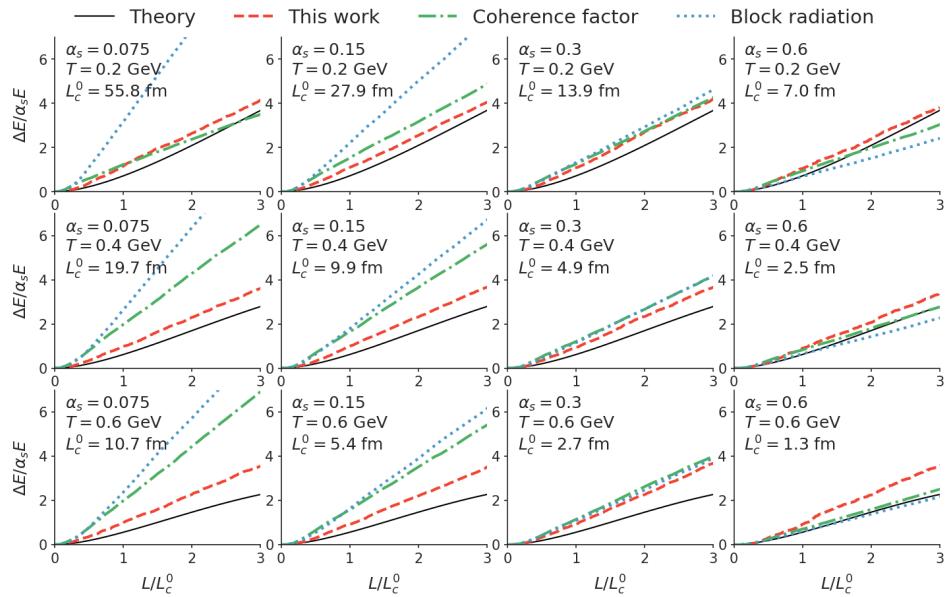


Figure 3.13 Energy loss ΔE as a function of path length L , temperature T and coupling constant α_s . Each column corresponds to a coupling constant of value $\alpha_s = 0.075, 0.15, 0.3$, and 0.6 (from left to right). Each row corresponds to a temperature of value $T = 0.2, 0.4$, and 0.6 GeV (from top to bottom). ΔE is scaled by $\alpha_s E$ and L is scaled by an estimated critical path length $L_c^0 = \sqrt{E/\hat{q}_0}$, $\hat{q}_0 = C_A \alpha_s T m_D^2$. The MC implementations in this work (red dashed lines) is compared to the ‘‘coherence factor’’ approach (green dash-dotted lines) and the ‘‘block radiation’’ approach (blue dotted lines). The analytic results for a thin medium are denoted as black solid lines.

Within each subplot, the parton energy varies from 10 GeV to 200 GeV. Different Monte Carlo implementations of the LPM effect are shown in colored lines, AMY NLL results are shown as black bands (we only integrate ω above the Debye mass to calculate the AMY energy loss). Without a surprise, the “modified approach” approach (red-dashed lines) reproduces the energy, temperature, and coupling constant dependence of AMY NLL energy loss very well. The “coherence factor” approach (blue-dash-dotted lines) has a similar energy and temperature dependence to that of the theoretical baseline; however, it systematically deviates from the baseline for different values of the coupling constant in a logarithmic manner. For the “block radiation” approaches, the deviations from the baseline regarding their α_s -dependence are even bigger and the energy dependence also gets worse, which is not surprising as we have discussed its problem.

Next we examine the path-length (L) dependence of the energy loss ΔE of a quark with an initial energy of $E = 200$ GeV in a finite medium in Figure 3.13. Again, each column uses a different coupling constant and each row uses a different temperature. The path length within each subplot is varied up to four times L_c^0 . Here $L_c^0 = \sqrt{E/\hat{q}_0}$ with $\hat{q}_0 = C_A \alpha_s T m_D^2$ estimating the critical path length below which one expects a clear non-linear path-length dependence. All three implementations show the non-linear increase of ΔE as function of L . The “modified Boltzmann” approach stays close to the theory calculations when $L < L_c^0$ for all cases, while the other two approaches deviate systematically as α_s is varied, similar to our previous findings for the energy-loss in the infinite matter case.

3.7 Few-body matrix-elements

This section provides the detailed $2 \leftrightarrow 2$ and $2 \leftrightarrow 3$ matrix-elements we used in the transport model. The $2 \leftrightarrow 2$ results are standard and we do not re-derive here. The $2 \leftrightarrow 3$ cross-sections are more complicated and a detailed derivation is attached to show the approximations we made for readers reference.

3.7.1 $2 \leftrightarrow 2$ processes

The two-body scatterings between quarks, anti-quarks and gluons are standard and we quote the results from existing references [111]. For a light parton scattering, we keep only \hat{t} -channel contribution, the \hat{s} and \hat{u} channel

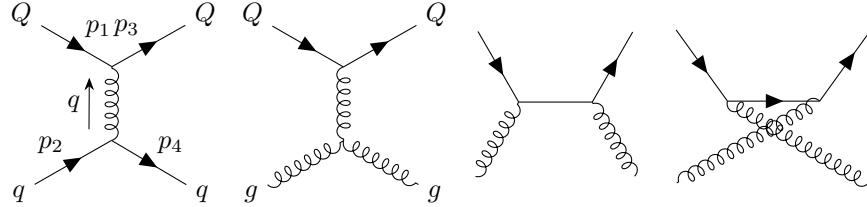


Figure 3.14 Elastic processes: The first diagram corresponds to heavy quark (Q) - light quark (q, \bar{q}) scattering. The last three diagrams contribute to heavy quark (Q) - gluon (g) scattering.

contribution are suppressed at high energy.

$$\overline{|M_{q_1 q_2 \rightarrow q_1 q_2}|^2} = \frac{64\pi^2 \alpha_s^2}{9} \frac{s^2 + u^2}{t^2} \quad (3.132)$$

$$\overline{|M_{gg \rightarrow gg}|^2} \approx 72\pi^2 \alpha_s^2 \frac{-su}{t^2} \quad (3.133)$$

$$\overline{|M_{qg \rightarrow qg}|^2} \approx 16\pi^2 \alpha_s^2 \frac{s^2 + u^2}{t^2} \quad (3.134)$$

For the heavy quark, since we are interested in its diffusion dynamics at low p_T , we uses the exact leading order matrix-element in the vacuum.

$$\begin{aligned} \overline{|M_{Qq \rightarrow Qq}|^2} &= \frac{64\pi^2 \alpha_s^2}{9} \frac{(M^2 - u)^2 + (s - M^2)^2 + 2M^2 t}{t^2} \\ \overline{|M_{Qq \rightarrow Qq}|^2} &= \pi^2 \left\{ 32\alpha_s^2 \frac{(s - M^2)(M^2 - u)}{t^2} \right. \\ &\quad + \frac{64}{9} \alpha_s^2 \frac{(s - M^2)(M^2 - u) + 2M^2(s + M^2)}{(s - M^2)^2} \\ &\quad + \frac{64}{9} \alpha_s^2 \frac{(s - M^2)(M^2 - u) + 2M^2(u + M^2)}{(M^2 - u)^2} \\ &\quad + \frac{16}{9} \alpha_s^2 \frac{M^2(4M^2 - t)}{(M^2 - u)(s - M^2)} \\ &\quad + 16\alpha_s^2 \frac{(s - M^2)(M^2 - u) + M^2(s - u)}{t(s - M^2)} \\ &\quad \left. - 16\alpha_s^2 \frac{(s - M^2)(M^2 - u) - M^2(s - u)}{t(M^2 - u)} \right\} \quad (3.135) \end{aligned}$$

3.7.2 $2 \rightarrow 3$ matrix-elements

Large-Q $2 \rightarrow 3$ inelastic processes are $g + i \rightarrow q + \bar{q} + i$, $q + i \rightarrow q + g + i$ and $g + i \rightarrow g + g + i$, where i stands for a medium parton, and the rest symbols stands for hard parton. In medium frame, hard parton has an energy $E \gg T$, while the medium thermal parton has $E \sim T$, and the typical center-of-mass energy is therefore $\sqrt{6ET}$. We perform the calculation in the the center-of-mass frame of the two incoming parton and let the hard parton to be moving towards the $+z$ direction with momentum p_1 , and the medium parton moving to the $-z$ direction with p_2 . The hard parton then splits into two daughter partons with momenta k and $p_1 + q - k$. The momentum transfer q between the hard parton and the medium parton is thought to be large enough $|q| > Q_{\text{cut}}$ so we neglect the thermal correction to its propagator.

Our derivation largely follows the work [77] while relaxing the soft approximation $xq_\perp \ll k_\perp$ in [77], and we only use the collinear approximation $k_\perp^2, q_\perp^2 \ll x(1-x)\hat{s}$ with $x = k^+/\sqrt{s} = k_\perp e_k^y/\sqrt{s}$. Also, we only include the contributions with a \hat{t} -channel momentum exchange between the medium and the hard partons. The collinear approximation requires $y_k \gg \ln(k_\perp/\sqrt{s})$ so that y_k cannot be arbitrarily small and $y_k > 0 >> -\ln(\sqrt{s}/k_\perp)$ is a reasonable range of application. Because $\hat{s} \sim 6ET$, we expect this approximation to break down when either the typical values of q_\perp^2 becomes comparable to $x(1-x)6ET$ or when $y_k < 0$ ($x < k_\perp/\sqrt{s} \sim k_\perp/\sqrt{6ET}$). We shall briefly mention the treatment of the $y_k < 0$ region in the end.

The light-cone momentum for p_1 , p_2 and k can written down directly using \sqrt{s} , x and k_\perp , then applying the above collinear condition, the expression for q (and therefore p_3 and p_4) is obtained by kinematic constraint up to corrections of order $\{k_\perp, q_\perp^2\}/x(1-x)\hat{s}$.

$$p_1 = (\sqrt{s}, 0, \vec{0}) \quad (3.136)$$

$$p_2 = (0, \sqrt{s}, \vec{0}) \quad (3.137)$$

$$k = (x\sqrt{s}, \frac{k_\perp^2}{x\sqrt{s}}, \vec{k}_\perp) \quad (3.138)$$

$$q \sim \left(-\frac{q_\perp^2}{\sqrt{s}}, \frac{q_\perp^2 + k_\perp^2/x - 2\vec{q}_\perp \cdot \vec{k}_\perp}{(1-x)\sqrt{s}}, \vec{k}_\perp \right) \quad (3.139)$$

Using the light-cone gauge with a light-like vector $n = (0, 1, 0)$, the gauge fixing condition $n \cdot A = 0$ eliminates the "+" component in the gluon (with momentum p) polarization vector, and is obtained by applying the transverse

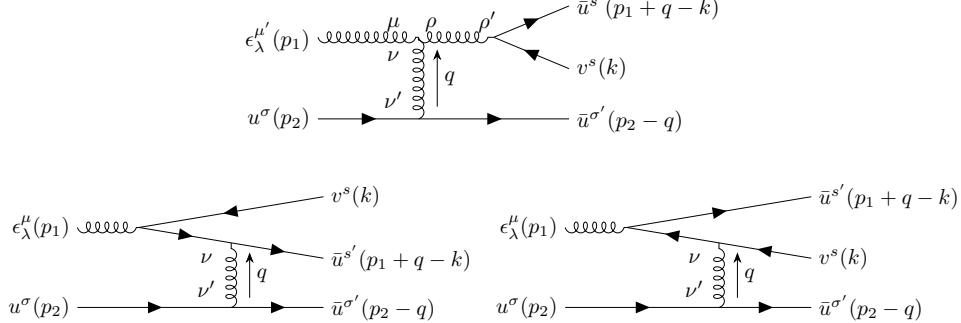


Figure 3.15 Three diagrams A (Top), B (Bottom left), C (Bottom right) that contribute to the large angle scattering induced gluon splitting into quark-anti-quark pair in the forward region of the center-of-mass frame.

condition $\epsilon \cdot p = 0$ (up to a higher order correction to its normalization)

$$\epsilon(p) \sim (0, \frac{2\vec{\epsilon}_\perp \cdot \vec{p}_\perp}{p^+}, \vec{\epsilon}_\perp). \quad (3.140)$$

With these preparations, the matrix-element is factorized into an amplitude for the splitting process (approximated in the collinear limit) times the amplitude for two-body collision with the medium parton. We shall only derive explicitly the cases where the medium parton is a quark, for colliding with medium anti-quark and gluon, it is sufficient to replace the $H + q \xrightarrow{\hat{t}} H + q$ amplitude by $H + \bar{q} \xrightarrow{\hat{t}} H + \bar{q}$ and $H + g \xrightarrow{\hat{t}} H + g$. The connect of these results to the Bethe-Heitler limit of the AMY integral equation will be elucidated in the end.

Gluon splitting to quark-anti-quark pair Three Feynman diagrams contribute to the kinematic region $y_k > 0$ in the current approximation, as shown in figure 3.15. We start from the amplitude for diagram A .

$$\begin{aligned} iM_A &= (-ig)^2 (-g) f^{abc}(t^b)_{j'j} (t^c)_{i'i} \epsilon_\lambda^\mu(p_1) \\ &\quad \frac{-i}{(p_1 + q)^2} \left(g^{\rho\rho'} - \frac{n^\rho(p_1 + q)^{\rho'} + n^{\rho'}(p_1 + q)^\rho}{n \cdot (p_1 + q)} \right) \bar{u}^s(p_1 + q - k) \gamma_{\rho'} v^{s'}(k) \\ &\quad \frac{-i}{q^2} \left(g^{\nu\nu'} - \frac{n^\nu q^{\nu'} + n^{\nu'} q^\nu}{n \cdot q} \right) \bar{u}^\sigma(p_4) \gamma_{\nu'} u^{\sigma'}(p_2) \\ &\quad [g_{\mu\nu}(p_1 - q)_\rho + g_{\nu\rho}(2q + p_1)_\rho + g_{\rho\mu}(-2p_1 - q)_\nu] \end{aligned} \quad (3.141)$$

Next, express the projection matrix of the gluon propagator with momentum $p_1 + q$ by the sum of tensor products of its polarization vectors, and

identify the amplitude $iP_{A,\lambda'}^{ss'}$ for a gluon with polarization λ' to split into the quark and anti-quark pair with spin s and s' . Also, use the high energy approximation to replace $\bar{u}^i(a)\gamma^\alpha u^j(b)$ by $(a+b)^\alpha \delta^{ij}$, then

$$iM_A \approx -g^3 f^{abc}(t^b)_{j'j}(t^c)_{i'i}\delta^{\sigma\sigma'}\epsilon^\mu(p_1) \quad (3.142)$$

$$\frac{1}{(p_1+q)^2} \sum_{\lambda'=\pm} \epsilon_{\lambda'}^\rho(p_1+q) \underbrace{\epsilon_{\lambda'}^{*\rho'}(p_1+q) \bar{u}^s(p_1+q-k) \gamma_{\rho'} v^{s'}(k)}_{iP_{A,\lambda'}^{ss'}}$$

$$\begin{aligned} & \frac{1}{q_\perp^2} \left(g^{\nu\nu'} - \frac{n^\nu q^{\nu'} + n^{\nu'} q^\nu}{n \cdot q} \right) (2p_2 - q)_\nu' \\ & [g_{\mu\nu}(p_1 - q)_\rho + g_{\nu\rho}(2q + p_1)_\rho + g_{\rho\mu}(-2p_1 - q)_\nu] \\ = & -g^3 f^{abc}(t^b)_{j'j}(t^c)_{i'i} \frac{1}{(p_1+q)^2} \frac{1}{q_\perp^2} \sum_{\lambda'=\pm} iP_{A,\lambda'}^{ss'} \delta^{\sigma\sigma'} \\ & \epsilon_\lambda^\mu(p_1) 2p_2^\nu \epsilon_{\lambda'}^\rho(p_1+q) [g_{\mu\nu}(p_1 - q)_\rho + g_{\nu\rho}(2q + p_1)_\rho + g_{\rho\mu}(-2p_1 - q)_\nu]. \end{aligned} \quad (3.143)$$

Finally, we evaluate the contraction in the second line using the expression for p_1, q and ϵ , and keep only terms that is leading in q_\perp^2/s to get,

$$iM_A \approx -g^3 f^{abc}(t^b)_{j'j}(t^c)_{i'i}\delta^{\sigma\sigma'} \frac{2s}{q_\perp^2} \frac{x(1-x)}{(\vec{k}_\perp - x\vec{q}_\perp)^2} iP_{A,\lambda}^{ss'}. \quad (3.144)$$

Diagram B and C are similar and we only write down diagram B in detail.

$$\begin{aligned} iM_B = & (-ig)^3 (t^b t^a)_{i'i} (t^b)_{j'j} \epsilon_\lambda^\mu(p_1) \quad (3.145) \\ & \frac{-i}{q^2} \left(g^{\nu\nu'} - \frac{n^\nu q^{\nu'} + n^{\nu'} q^\nu}{n \cdot q} \right) \\ & \bar{u}^s(p_1 + q - k) \gamma_\nu \frac{i(p_1 - k)}{(p_1 - k)^2} \gamma^\mu v^{s'}(k) \\ & \bar{u}^\sigma(p_4) \gamma_{\nu'} u^{\sigma'}(p_2) \end{aligned}$$

Again, represent the tensor structure of the fermion propagator by the sum of tensor products of the spinors, identify the splitting amplitude $iP_{B,\lambda'}^{ss'}$ and

use the high energy limit of the current,

$$iM_B \approx ig^3(t^b t^a)_{i'i}(t^b)_{j'j} \quad (3.146)$$

$$\begin{aligned} & \frac{-i}{q_\perp^2} \left(g^{\nu\nu'} - \frac{n^\nu q^{\nu'} + n^{\nu'} q^\nu}{n \cdot q} \right) (2p_2 - q)_\nu' \\ & \frac{1}{2p_1 \cdot k} \sum_\sigma \bar{u}^s(p_1 + q - k) \gamma_\nu u^\sigma(p_1 - k) \underbrace{\epsilon_\lambda^\mu(p_1) \bar{u}^\sigma(p_1 - k) \gamma^\mu v^{s'}(k)}_{iP_{B,\lambda}^{\sigma s'}} \end{aligned}$$

$$\begin{aligned} & \approx ig^3(t^b t^a)_{i'i}(t^b)_{j'j} \frac{-i}{q_\perp^2} \frac{1}{2p_1 \cdot k} iP_{B,\lambda}^{ss'} \\ & \left(g^{\nu\nu'} - \frac{n^\nu q^{\nu'} + n^{\nu'} q^\nu}{n \cdot q} \right) (2p_2 - q)_\nu' (2p_1 - q + 2k)_\nu \end{aligned} \quad (3.147)$$

Note that iP_B is different from iP_A as the initial splitting parton has a different transverse momentum from diagram A . Finally, evaluate the contraction and get,

$$iM_B = ig^3(t^b t^a) i' i t^b j' j \delta^{\sigma\sigma'} \frac{2s}{q_\perp^2} \frac{x(1-x)}{k_\perp^2} iP_{B,\lambda}^{ss'} \quad (3.148)$$

Diagram C can be obtained similarly,

$$iM_C = -ig^3(t^a t^b) i' i t^b j' j \delta^{\sigma\sigma'} \frac{2s}{q_\perp^2} \frac{x(1-x)}{(\vec{k}_\perp - \vec{q}_\perp)^2} iP_{C,\lambda}^{ss'} \quad (3.149)$$

To sum the contributions from all three diagrams, applying $f^{abc}t^c = -i[t^a, t^b]$ to iM_A and the result is,

$$\begin{aligned} i(M_A + M_B + M_C) &= ig^3 \frac{2s}{q_\perp^2} (t^b)_{j'j} x(1-x) \\ & \left\{ (t^a t^b)_{i'i} \left(\frac{iP_{A,\lambda}^{ss'}}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{iP_{C,\lambda}^{ss'}}{(\vec{k}_\perp - \vec{q}_\perp)^2} \right) \right. \\ & \left. - (t^a t^b)_{i'i} \left(\frac{iP_{A,\lambda}^{ss'}}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{iP_{B,\lambda}^{ss'}}{k_\perp^2} \right) \right\} \end{aligned} \quad (3.150)$$

Now we have to address what those splitting amplitudes are. Label the four momenta as $p_g = c$, $p_q = a$, $p_{\bar{q}} = b$. And use the following representation for the spinors,

$$u^s(p) = (\sqrt{p \cdot \sigma} \xi^s, \sqrt{p \cdot \bar{\sigma}} \xi^s)^T v^s(p) = (\sqrt{p \cdot \sigma} \eta^s, -\sqrt{p \cdot \bar{\sigma}} \eta^s)^T \quad (3.151)$$

where $\sigma_{i=\{1,2,3\}}$ are Pauli matrices, $\sigma = (1_{2 \times 2}, \vec{\sigma})$, and $\bar{\sigma} = (1_{2 \times 2}, -\vec{\sigma})$. The square root of the matrix is,

$$\sqrt{p \cdot \sigma} = \begin{bmatrix} p^- & -p_L^\perp \\ -p_R^\perp & p^+ \end{bmatrix}^{1/2} = \frac{1}{\sqrt{2(E \pm M)}}(p \cdot \sigma \pm \mathbf{1}M) \quad (3.152)$$

$$\sqrt{p \cdot \bar{\sigma}} = \begin{bmatrix} p^+ & p_\perp^- \\ p_R^\perp & p^- \end{bmatrix}^{1/2} = \frac{1}{\sqrt{2(E \pm M)}}(p \cdot \bar{\sigma} \pm \mathbf{1}M) \quad (3.153)$$

$$(3.154)$$

where M is the mass of the particle, $p^\pm = E \pm p_z$, and $p_{R,L}^\perp = p_x \pm ip_y$. Currently, we only consider the massless case, because the mass effect is not implemented in the few-body matrix-elements in our model. Neglecting the mass, the splitting amplitude is,

$$\epsilon_{\lambda,\mu}(c)\bar{u}_s(a)\gamma^\mu v_{s'}(b) \quad (3.155)$$

$$= \frac{1}{\sqrt{2a}\sqrt{2b}}(\xi_s^T a \cdot \sigma, \xi_s^T a \cdot \bar{\sigma}) \begin{bmatrix} \epsilon \cdot \bar{\sigma} & 0 \\ 0 & \epsilon \cdot \sigma \end{bmatrix} \begin{bmatrix} b \cdot \sigma \eta_{s'} \\ b \cdot \bar{\sigma} \eta_{s'} \end{bmatrix} \quad (3.156)$$

$$= \frac{1}{2\sqrt{ab}}\xi_s^T \begin{bmatrix} a^- & -a_L^\perp \\ -a_R^\perp & a^+ \end{bmatrix} \begin{bmatrix} 0 & \sqrt{2}\delta_{\lambda L} \\ \sqrt{2}\delta_{\lambda R} & \frac{\sqrt{2}c_\lambda^\perp}{c^+} \end{bmatrix} \begin{bmatrix} b^- & -b_L^\perp \\ -b_R^\perp & b^- \end{bmatrix} \eta_{s'} \quad (3.157)$$

$$- \frac{1}{2\sqrt{ab}}\xi_s^T \begin{bmatrix} a^+ & a_L^\perp \\ a_R^\perp & a^- \end{bmatrix} \begin{bmatrix} \frac{\sqrt{2}c_\lambda^\perp}{c^+} & -\sqrt{2}\delta_{\lambda R} \\ -\sqrt{2}\delta_{\lambda L} & 0 \end{bmatrix} \begin{bmatrix} b^+ & b_L^\perp \\ b_R^\perp & b^- \end{bmatrix} \eta_{s'}$$

$$= \frac{1}{\sqrt{2ab}}\xi_s^T \begin{bmatrix} -a_L^\perp b^- \delta_{\lambda L} - a^- b_L^\perp \delta_{\lambda R} + a_L^\perp b_R^\perp \frac{c_\lambda^\perp}{c^+} & a_L^\perp b_L^\perp \delta_{\lambda L} + a^- b^+ \delta_{\lambda R} - a_L^\perp b^+ \frac{c_\lambda^\perp}{c^+} \\ a^+ b^- \delta_{\lambda L} + a_R^\perp b_L^\perp \delta_{\lambda R} - a^+ b_R^\perp \frac{c_\lambda^\perp}{c^+} & -a^+ b_L^\perp \delta_{\lambda L} - a_R^\perp b^+ \delta_{\lambda R} + a^+ b^+ \frac{c_\lambda^\perp}{c^+} \end{bmatrix} \quad (3.158)$$

$$- \frac{1}{\sqrt{2ab}}\xi_s^T \begin{bmatrix} -a_L^\perp b^+ \delta_{\lambda L} - a^+ b_R^\perp \delta_{\lambda R} + a^+ b^+ \frac{c_\lambda^\perp}{c^+} & -a_L^\perp b_L^\perp \delta_{\lambda L} - a^+ b^- \delta_{\lambda R} + a^+ b_L^\perp \frac{c_\lambda^\perp}{c^+} \\ -a^- b^+ \delta_{\lambda L} - a_R^\perp b_L^\perp \delta_{\lambda R} + a_R^\perp b^+ \frac{c_\lambda^\perp}{c^+} & -a^- b_L^\perp \delta_{\lambda L} - a_R^\perp b^- \delta_{\lambda R} + a_R^\perp b_L^\perp \frac{c_\lambda^\perp}{c^+} \end{bmatrix} \eta_{s'}$$

Keep the leading terms in the collinear limit which are products of (+)(+) or (+)(\perp) components of the momenta, and drop terms that are of order (+)(-), (\perp)(\perp) and (\perp)(-),

$$\epsilon_{\lambda,\mu}\bar{u}_s(a)\gamma^\mu v_{s'}(b) \quad (3.159)$$

$$= \frac{1}{\sqrt{2ab}}\xi_s^T \begin{bmatrix} a_L^\perp b^+ \delta_{\lambda L} + a^+ b_R^\perp \delta_{\lambda R} - a^+ b^+ \frac{c_\lambda^\perp}{c^+} & 0 \\ 0 & -a^+ b_L^\perp \delta_{\lambda L} - a_R^\perp b^+ \delta_{\lambda R} + a^+ b^+ \frac{c_\lambda^\perp}{c^+} \end{bmatrix} \quad (3.160)$$

There are four combinations for the possible initial state polarization and

final state spins

$$\epsilon_{\lambda,\mu} \bar{u}_s(a) \gamma^\mu v_{s'}(b) = \frac{x\vec{a} - (1-x)\vec{b}}{\sqrt{2x(1-x)}} \begin{cases} x, & \lambda = L, s = \uparrow \\ -(1-x), & \lambda = L, s = \downarrow \\ (1-x), & \lambda = R, s = \uparrow \\ -x, & \lambda = R, s = \downarrow \end{cases} \quad (3.161)$$

Where we have use $a^+ = (1-x)c^+, b^+ = xc^+$ and $c_\perp = a_\perp + b_\perp$. Sum over the spins and average over polarization for the squared amplitude,

$$\frac{1}{2} \sum_{\pm} |P|^2 = \frac{2(x^2 + (1-x)^2)}{x(1-x)} \left((1-x)\vec{a}_\perp - x\vec{b}_\perp \right)^2. \quad (3.162)$$

This result goes back to the standard splitting function if it is computed in the frame where $a_\perp = -b_\perp$. However, there is no such frame that $a_\perp = -b_\perp$ satisfies simultaneously for the splitting in diagram A, B and C, therefore different amplitude needs to be inserted for each diagram and we find,

$$\frac{\sum_{\lambda,s,s',\sigma,\sigma',a,b} |M^2|_{g+q \rightarrow q+\bar{q}+q}}{2d_F 2d_A} = g^4 \frac{2C_F}{d_A} \frac{4s^2 x(1-x)}{q_\perp^4} \times g^2 \frac{(x^2 + (1-x)^2)}{2} \left(C_F \vec{A}^2 + C_F \vec{B}^2 - (2C_F - C_A) \vec{A} \cdot \vec{B} \right) \quad (3.163)$$

Where the \vec{A} and \vec{B} is,

$$\vec{A} = \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2}, \quad (3.164)$$

$$\vec{B} = \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{\vec{k}_\perp}{\vec{k}_\perp^2}. \quad (3.165)$$

The final squared matrix-element has been factorized into the two body scattering part (first line) and the collinear splitting part (second line) with the desired leading order QCD splitting function.

Quark splits to quark and gluon The Feynman diagrams to be included for $q + q \rightarrow q + g + q$ are shown in Figure 3.16. The calculation uses exactly the same technique we used for the gluon splitting channel, and we

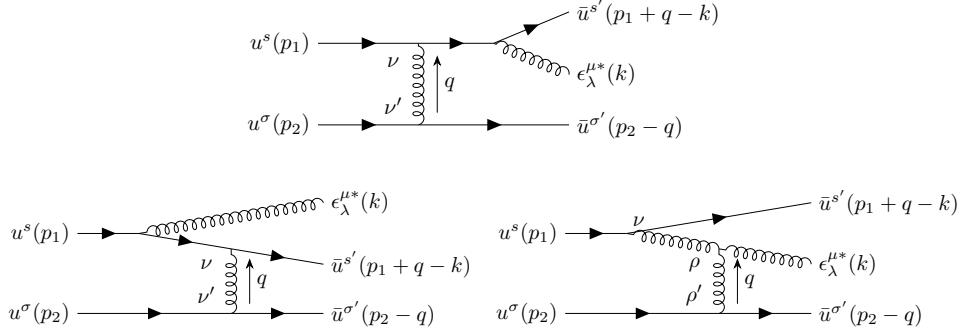


Figure 3.16 Three diagrams A (Top), B (Bottom left), C (Bottom right) that contribute to the large angle scattering induced a quark splitting into a quark and a gluon in the forward region of the center-of-mass frame.

present the result directly,

$$\overline{|M^2|}_{g+q \rightarrow g+g+q} = g^4 \frac{C_F}{d_F} \frac{4s^2}{q_\perp^4} x(1-x) \times g^2 \frac{1+(1-x)^2}{x} (C_F \vec{A}^2 + C_F \vec{B}^2 - (2C_F - C_A) \vec{A} \cdot \vec{B}) \quad (3.166)$$

$$\vec{A} = \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2} - \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2} \quad (3.167)$$

$$\vec{B} = \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2} - \frac{\vec{k}_\perp}{\vec{k}_\perp^2} \quad (3.168)$$

Gluon splitting to two gluons Finally, for $g + q \rightarrow g + q + g$, the Feynman diagrams are shown in Figure 3.17. The simplification of the two body collision amplitude can be done in a similar manner as the previous two channels. We only write down the splitting amplitude $g \rightarrow g + g$ in detail. Suppressing the color index, we label the initial gluon with $\epsilon_1^\mu(p)$, and the two daughter gluons with $\epsilon_2^\nu(k)$ and $\epsilon_3^\rho(q)$. The splitting amplitudes

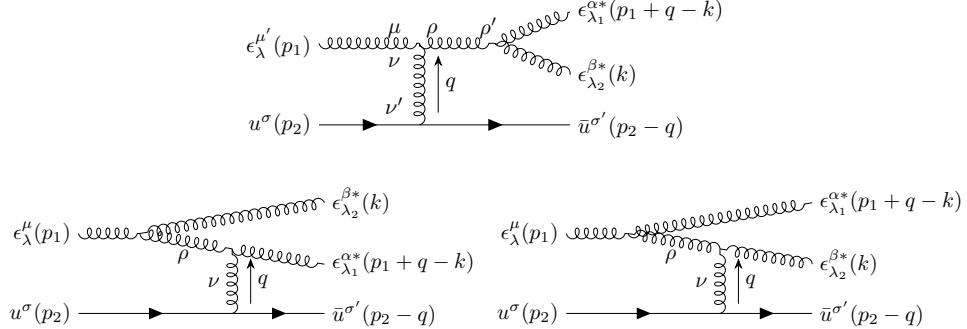


Figure 3.17 Three diagrams A (Top), B (Bottom left), C (Bottom right) that contribute to the large angle scattering induced gluon splitting into two gluons in the forward region of the center-of-mass frame.

are then (omitting the factor $-gf^{abc}$)

$$iP = \epsilon_1^\mu \epsilon_2^\nu \epsilon_3^\rho [g_{\mu\nu}(p+k)_\rho + g_{\nu\rho}(p+k)_\mu + g_{\rho\mu}(-q-p)_\nu] \quad (3.169)$$

$$= -\vec{\epsilon}_{1,\perp} \cdot \vec{\epsilon}_{2,\perp} \left[(p+k)^+ \frac{\vec{\epsilon}_{3,\perp} \cdot \vec{q}_\perp}{q^+} - \vec{\epsilon}_{3,\perp} \cdot (\vec{p}_\perp + \vec{k}_\perp) \right] \quad (3.170)$$

$$\begin{aligned} & -\vec{\epsilon}_{2,\perp} \cdot \vec{\epsilon}_{3,\perp} \left[(-k+q)^+ \frac{\vec{\epsilon}_{1,\perp} \cdot \vec{p}_\perp}{p^+} - \vec{\epsilon}_{1,\perp} \cdot (-\vec{k}_\perp + \vec{q}_\perp) \right] \\ & -\vec{\epsilon}_{3,\perp} \cdot \vec{\epsilon}_{1,\perp} \left[(-q-p)^+ \frac{\vec{\epsilon}_{2,\perp} \cdot \vec{k}_\perp}{k^+} - \vec{\epsilon}_{2,\perp} \cdot (-\vec{q}_\perp - \vec{p}_\perp) \right] \end{aligned}$$

There are four possible combinations of the polarization vectors, and their respective amplitude is computed as,

$$iP = \sqrt{2} \left[x \vec{q}_\perp - (1-x) \vec{k}_\perp \right] \times \begin{cases} \frac{1-x+x^2}{x(1-x)}, & \lambda_1 = \lambda_2 = \lambda_3 \\ -1, & \lambda_1 \neq \lambda_2 = \lambda_3 \\ \frac{1}{x}, & \lambda_1 = \lambda_3 \neq \lambda_2 \\ \frac{1}{1-x}, & \lambda_1 = \lambda_2 \neq \lambda_3 \end{cases} \quad (3.171)$$

Summing over the squared amplitude of all four cases and average over the initial gluon polarization, one gets the desired leading order QCD splitting function,

$$2 \frac{1+x^2+(1-x)^4}{x^2(1-x)^2} \left[x \vec{q}_\perp - (1-x) \vec{k}_\perp \right]^2. \quad (3.172)$$

Substitute the the amplitude in each diagram, the final squared matrix-element is

$$\overline{|M^2|}_{g+q \rightarrow g+g+q} = g^4 \frac{C_A}{d_F} \frac{4s^2 x(1-x)}{q_\perp^4} \quad (3.173)$$

$$\times g^2 \frac{1+x^4 + (1-x)^4}{x(1-x)} (C_A \vec{A}^2 + C_A \vec{B}^2 - C_A \vec{A} \cdot \vec{B})$$

$$\vec{A} = \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2} \quad (3.174)$$

$$\vec{B} = \frac{\vec{k}_\perp - x\vec{q}_\perp}{(\vec{k}_\perp - x\vec{q}_\perp)^2} - \frac{\vec{k}_\perp}{\vec{k}_\perp^2} \quad (3.175)$$

Regulating the $2 \rightarrow 3$ squared matrix-elements The divergence in the q integration is removed by the requirement that this few-body matrix-element only applies to processes with $q > Q_{\text{cut}}$. The collinear divergence when k approaching q , xq is regulated by including a gluon thermal mass. In practice, these collinear region will be further suppressed by the LPM effect. The cross-section is obtained by integrating over the final state phase-space, where we have chosen to parameterize the three particle final state in terms of k_\perp^2 , the rapidity of k in the center-of-mass frame y_k , and the solid angle of the recoil medium particle.

Soft limit: the Gunion-Bertsch approximation The result we obtained for the $g \rightarrow g + g$ and $q \rightarrow q + g$ channel has a soft limit that goes back to the well known Gunion-Bertsch form. By soft limit, we require the radiated gluon energy to be small enough such that $xq_\perp \ll k_\perp$. Then, the splitting amplitudes for both $g \rightarrow g + g$ and $q \rightarrow q + g$ are simplified into the same form,

$$\overline{|M|}_{22}^2 x(1-x) g^2 \frac{2(1-x + O(x^2))}{x} C_A \left(\frac{\vec{k}_\perp}{k_\perp^2} - \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2} \right)^2 \quad (3.176)$$

Neglecting the $O(x^2)$ terms in the splitting function, the result is the same as the improved verison of the Gunion-Bertsch cross-section [77] used in the full Boltzmann partonic transport model BAMPS [92],

$$\overline{|M|}_{22}^2 8\pi C_A \alpha_s (1-x)^2 \left(\frac{\vec{k}_\perp}{k_\perp^2} - \frac{\vec{k}_\perp - \vec{q}_\perp}{(\vec{k}_\perp - \vec{q}_\perp)^2} \right)^2 \quad (3.177)$$

The backward ($y_k < 0$) region We have mentioned in the beginning of the derivation that the condition $k_\perp^2 < x(1-x)\hat{s}$ restricts the splitting to be happen only for the parton moving in the $+z$ direction in the center-of-mass frame ($y_k > 0$). For splitting that happens in the backward region, another set of diagrams contributes, where the splitting comes from the parton that moves in the $-z$ direction in the center-of-mass frame. Also one needs a different gauge $A^- = 0$. The derivation is similar to the previous ones, but with the definition of x and q changed to $x = k^-/\sqrt{s}$, and $q = p_1 - p_3$.

To combine the results that is obtained in different regions of phase space ($y_k > 0$ and $y_k < 0$), we follow [77] and defines,

$$\bar{x} = \frac{(k + |k_z|)}{\sqrt{s}} = \frac{k_\perp e^{|y_k|}}{\sqrt{s}} \quad (3.178)$$

$$\bar{q} = \Theta(y_k)(p_2 - p_4) + \Theta(-y_k)(p_1 - p_3) \quad (3.179)$$

which replaces the original x and q in our formula, and the resultant matrix-elements can be used for both forward and backward regions.

Relation to the Bethe-Heitler limit of the AMY formalism Now we show the connection between the $2 \rightarrow 3$ cross section obtained here and the Bethe-Heitler limit of the AMY equation. In the Bethe-Heitler limit, the AMY integral equation can be solved approximately by treating $1/\tau_f$ as the leading factor. One get the splitting rate for each different channels (denoting \vec{a}/a^2 as $\vec{\phi}_a$),

$$R_{q \rightarrow q+g}^{BH} \propto g^2 P_{qg}^{q(0)}(x) \int dk^2 dq^2 \mathcal{A}(q^2) \left\{ C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k-q}) + (2C_F - C_A) \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+xq}) + C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+(1-x)q}) \right\} \quad (3.180)$$

$$R_{g \rightarrow g+g}^{BH} \propto g^2 P_{gg}^{g(0)}(x) \int dk^2 dq^2 \mathcal{A}(q^2) \left\{ C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k-q}) + C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+xq}) + C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+(1-x)q}) \right\} \quad (3.181)$$

$$R_{g \rightarrow q+\bar{q}}^{BH} \propto g^2 P_{q\bar{q}}^{g(0)}(x) \int dk^2 dq^2 \mathcal{A}(q^2) \left\{ (2C_F - C_A) \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k-q}) + C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+xq}) + C_A \vec{\phi}_k \cdot (\vec{\phi}_k - \vec{\phi}_{k+(1-x)q}) \right\} \quad (3.182)$$

with the collision kernel $\mathcal{A} = g^2 T m_D^2 / q^2 (q^2 + m_D^2)$. These expression looks drastically different from the incoherent rate computed using the cross-section derived in the previous section, however, we would like to show that they are the same once integration over dk^2 is performed. Therefore,

the incoherent rate we used in the Boltzmann equation indeed recover the Bethe-Heitler limit of the AMY integral equation.

To show this, we start from the $2 \rightarrow 3$ rate formula using the matrix-elements from equation. Starting from the $q \rightarrow q + g$ channel, the rate in our Boltzmann equation is,

$$\begin{aligned} R_{q \rightarrow q+g} &\propto g^2 P_{qg}^{q(0)}(x) \int \frac{f(p_2) dp_2^3}{2E_2(2\pi)^3} dq^2 \frac{g^4}{q^4} \\ &\quad \int dk^2 \left\{ C_F \left(\vec{\phi}_{k-q} - \vec{\phi}_{k-xq} \right)^2 + C_F \left(\vec{\phi}_{k-q} - \vec{\phi}_k \right)^2 \right. \\ &\quad \left. - (2C_F - C_A) \left(\vec{\phi}_{k-q} - \vec{\phi}_{k-xq} \right) \cdot \left(\vec{\phi}_{k-q} - \vec{\phi}_k \right) \right\} \end{aligned} \quad (3.183)$$

Focusing on the three products (squares) of $\vec{\phi}$ s under the dk^2 integration, we are going to expand the first term in each product and then shift the argument of the first $\vec{\phi}$ to k ,

$$\begin{aligned} R_{q \rightarrow q+g} &\propto g^2 P_{qg}^{q(0)}(x) \int \frac{f(p_2) dp_2^3}{2E_2(2\pi)^3} dq^2 \frac{g^4}{q^4} \\ &\quad \int dk^2 \left\{ C_F \vec{\phi}_k \left(\vec{\phi}_k - \vec{\phi}_{k+(1-x)q} \right) - C_F \vec{\phi}_k \left(\vec{\phi}_{k-(1-x)q} - \vec{\phi}_k \right) \right. \\ &\quad + C_F \vec{\phi}_k \left(\vec{\phi}_k - \vec{\phi}_{k+q} \right) - C_F \vec{\phi}_k \left(\vec{\phi}_{k-q} - \vec{\phi}_k \right) \\ &\quad \left. - (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+q} \right) + (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_{k-(1-x)q} - \vec{\phi}_{k+xq} \right) \right\} \end{aligned} \quad (3.184)$$

Next, flip the sign of q under the integration, and meanwhile, insert a $-\vec{\phi}_k + \vec{\phi}_k$ in the brackets of the last term,

$$\begin{aligned} R_{q \rightarrow q+g} &\propto g^2 P_{qg}^{q(0)}(x) \int \frac{f(p_2) dp_2^3}{2E_2(2\pi)^3} dq^2 \frac{g^4}{q^4} \\ &\quad \int dk^2 \left\{ 2C_F \vec{\phi}_k \left(\vec{\phi}_k - \vec{\phi}_{k+(1-x)q} \right) + 2C_F \vec{\phi}_k \left(\vec{\phi}_k - \vec{\phi}_{k+q} \right) \right. \\ &\quad - (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+q} \right) + (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_{k+(1-x)q} - \vec{\phi}_k \right) \\ &\quad \left. + (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+xq} \right) \right\} \end{aligned} \quad (3.185)$$

After this manipulation, the first (second) term cancels the C_F part of the fourth (third) term,

$$\begin{aligned} R_{q \rightarrow q+g} &\propto g^2 P_{qg}^{q(0)}(x) \int \frac{f(p_2) dp_2^3}{2E_2(2\pi)^3} dq^2 \frac{g^4}{q^4} \\ &\quad \int dk^2 \left\{ C_A \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+q} \right) + C_A \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+(1-x)q} \right) \right. \\ &\quad \left. + (2C_F - C_A) \vec{\phi}_k \cdot \left(\vec{\phi}_k - \vec{\phi}_{k+xq} \right) \right\} \end{aligned} \quad (3.186)$$

which is the same integration as the one obtained from the Bethe-Heitler limit of the AMY equation (neglecting the screen mass in \mathcal{A} when $q^2 \gg m_D^2$) The equivalence between these two expressions of the $g \rightarrow g + g$ channel and the $g \rightarrow q + \bar{q}$ channel can also be shown similarly.

Mass effect in the $2 \rightarrow 3$ squared matrix-elements For completeness, we briefly outline the derivation of $2 \rightarrow 3$ cross-section with mass effect. As a remark, putting heavy flavor mass directly into the these matrix-elements are certainly legitimate if one only focus on $2 \rightarrow 3$ processes. But once we want to approximate the effect of multiple scatterings: $(n \rightarrow n+1) \approx (2 \rightarrow 3)(2 \rightarrow 2) \cdots (2 \rightarrow 2) \times$ corrections, it is not advantages to put the mass effect into the $(2 \rightarrow 3)$ part, but into the last step of corrections, which is the approach we used.

First, we still work under the assumption that $M \ll E$, and will only keep terms when M is making direct comparison to k_\perp, q_\perp . The kinematics are now changed to,

$$p_1 = (\sqrt{s}, 0, \vec{0}) \quad (3.187)$$

$$p_2 = (0, \sqrt{s}, \vec{0}) \quad (3.188)$$

$$k = (x\sqrt{s}, \frac{k_\perp^2}{x\sqrt{s}}, \vec{k}_\perp) \quad (3.189)$$

$$q \sim \left(-\frac{q_\perp^2 \sqrt{s}}{s - M^2}, \frac{x(\vec{q}_\perp - \vec{k}_\perp)^2 + (1-x)k_\perp^2 + x^2 M^2}{x(1-x)\sqrt{s}}, \vec{k}_\perp \right) \quad (3.190)$$

For the splitting amplitude, off diagonal elements of $\epsilon_{\lambda,\mu}(c)\bar{u}_s(a)\gamma^\mu v_{s'}(b)$ also needs to be included for helicity flipping process. Moreover,

$$\sqrt{p \cdot \sigma} = \frac{p \cdot \sigma + M}{\sqrt{2(E+M)}} \approx \frac{p \cdot \sigma + M}{\sqrt{2E}} \quad (3.191)$$

$$\sqrt{p \cdot \bar{\sigma}} = \frac{p \cdot \bar{\sigma} + M}{\sqrt{2(E+M)}} \approx \frac{p \cdot \bar{\sigma} + M}{\sqrt{2E}} \quad (3.192)$$

where we have omitted the mass in the denominator since it only involves corrections of order M/E . From this one can see that the previous calculation can be used for the massive case with the substitution $a^\pm \rightarrow a^\pm + M$

and $b^\pm \rightarrow b^\pm + M$. Then, the splitting amplitude becomes,

$$\epsilon_{\lambda,\mu} \bar{u}_s(a) \gamma^\mu v_{s'}(b) = \frac{1}{\sqrt{2ab}} \xi_s^T A_{ss'} \eta_{s'} \quad (3.193)$$

$$A_{\uparrow\uparrow} = \delta_{\lambda L} 2b_z a_L^\perp + \delta_{\lambda R} 2a_z b_R^\perp + \frac{c_\lambda^\perp}{c^+} (a_L^\perp b_R^\perp - a^+ b^+) \quad (3.194)$$

$$A_{\downarrow\downarrow} = -\delta_{\lambda L} 2a_z b_L^\perp - \delta_{\lambda R} 2b_z a_R^\perp - \frac{c_\lambda^\perp}{c^+} (a_R^\perp b_L^\perp - a^+ b^+) \quad (3.195)$$

$$A_{\uparrow\downarrow} = \delta_{\lambda L} 2a_L^\perp b_L^\perp + \delta_{\lambda R} (a^+ b^- + a^- b^+) - \frac{c_\lambda^\perp}{c^+} (a^+ b^\perp + (3.196))$$

$$A_{\downarrow\uparrow} = \delta_{\lambda L} (a^+ b^- + a^- b^+) + \delta_{\lambda R} 2a_R^\perp b_R^\perp - \frac{c_\lambda^\perp}{c^+} (a^+ b^\perp + (3.197))$$

4

Comprehensive heavy-flavor simulation framework

The simulation framework for heavy flavor particles is summarized in the follow chart in figure 4.1. The soft initial condition model provide both the initial energy density of the medium and the transverse location of the hard vertices, while pQCD based calculations initialize the momentum space of the hard partons. The left branch of this flow chart – the hydrodynamic-based medium evolution model – in chapter 2. We briefly review of the right branch – the mutli-stage model for heavy-falvor. The hard production model is introduced in section 4.1. The initially produced partons are highly virtual and undergo the DGLAP evolution (vacuum shower) that bring down the virtuality; eventually at some point this evolution will be matched to the in-medium transport calculations. There is a complication for vacuum-like parton shower in a medium, since certain vacuum parton branchings would have occupied the same space-time as the medium and also receives medium corrections. Another obstacle is that multiple emissions are treated very differently between vacuum-like shower and medium-induce shower. For the vacuum evolution, the “time” variable is the virtuality scale with the space-time information integrated out, while the transport model evolves the systems in real time, with virtuality integrated out below a certain scale. There are many recent progress in both theory developments and newly design event-generators to solve this problem [112–118]. In section 4.2.1, we discuss a possible prescription to interface the two types of showers in our simulation. Section 4.3 contains the details of coupling the transport model to a dynamically evolving medium with large longitudinal expansion. The heavy flavor hadronization model and hadronic rescatterings are introduced

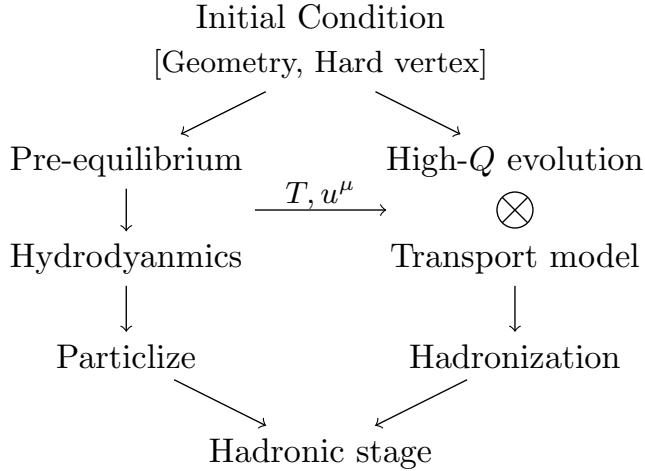


Figure 4.1 A schematic workflow of the heavy quark simulation. The left branch evolves the medium in the hydrodynamic based model, providing medium information (temperature, flow velocity) to the hard probe transport in the right branch. The hard and soft hadrons are evolved in the hadronic afterburner in the last step.

in section 4.4. The hadronization routine applies a previously implementation [107] of the high- p_T fragmentation plus low- p_T recombination model for heavy hadrons production [119]. Finally, in section 4.5, the model is benchmarked using a few choices of fixed coupling constant and running coupling constants, before being systematically tuned to data in the next chapter.

4.1 Initial production of heavy flavor

4.1.1 Factorization framework in proton-proton collisions

In the proton-proton collision, the hard processes can be computed using the pQCD-based techniques. The foundation of this calculation is the factorization framework as schematically demonstrated in 4.2. First, the incoming proton is a composite object and there is a certain ‘‘probability’’ of finding a parton $i(j)$ carrying $x_i(x_j)$ fraction of the momentum of the proton $p_1(p_2)$. This ‘‘probability’’ is known as the parton distribution function (PDF) $f_i(x, Q^2)$. It not only is a function of x , but also depends on the scale Q^2 at which the proton is probed. The probing scale is required to be much greater than the non-perturbative scale. Because $\alpha_s(Q^2)$ is small due to

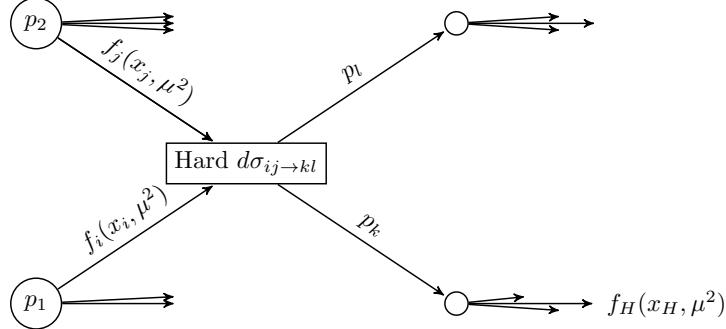


Figure 4.2 A schematic demonstration of the factorization theorem. Two incoming proton momenta are p_1 and p_2 . $f_{i,j}$ are the parton distribution function. $d\sigma$ is the perturbative matrix-element. f_H is the fragmentation function.

asymptotic freedom, the process of partons i and j scatterings into partons k and l is computable in perturbative QCD. The final states partons eventually produce a bunch of hadrons, which is non-perturbative process. The parton fragmentation function is then defined as the probability to find a certain hadron H carrying a fraction x_H of the parton's momentum. Combining these pieces together, the cross-section for the inclusive production of hadron can be written as [120],

$$\frac{d\sigma_{p+p \rightarrow H+X}}{dy d\mathbf{p}_T^2} = \frac{1}{\pi} \int dx_i dx_j f_i(x_i, Q^2) f_j(x_j, Q^2) \frac{d\sigma_{ij \rightarrow kl}}{d\hat{t}} \frac{1}{z_k} D^H(z_k, Q^2). \quad (4.1)$$

Although the parton distribution function f and the parton fragmentation function D are essentially non-perturbative objects, they parametrizes universal long-distance physics and can be extracted from independent experiments at certain scales Q_0^2 . Moreover, the evolution from their “definition” scale Q_0^2 to the process scale Q^2 can be described by the DGLAP evolution equation [121–123] based on perturbative QCD to increase the predictive power of the factorization formula.

The DGLAP evolution takes into account that the initial high-virtuality parton i (or j) could have come from a splitting process of a parton with lower virtuality parton i' (or j'). Similarly, the final state high virtuality parton k (or l) could also split into a low virtuality parton k' (or l') before it turns into a hadron. Though each splitting causes an additional power of α_s , it is also magnified by a potentially large factor $\ln Q^2/\mu^2$ when the Q^2 is much greater than the scale where the f , D are defined. The same argument also applies to partons i', j', k', l' . The DGLAP equations sys-

tematically resum contributions including an arbitrary number of parton splittings and evolve the scale from μ^2 to the hard scale Q^2 . Moreover, a very useful parton-shower picture can be built from this process and with a probabilistic interpretation of the DGLAP evolution. Using Monte Carlo technique, one can even mimic the exclusive final states from the sequence of parton branching processes.

4.1.2 Production in the nuclear environment

The above framework explains very well explains the hard process production in the proton-proton collisions. In the nuclear environment, there are several differences. First, the parton distribution function inside a nuclei is different from the superposition of the nucleons. The ratio between nuclear PDF and proton PDF generally deviates from unity. In particular, this ratio for small x gluon is significantly below one, known as the nuclear shadowing effect. This ratio increase and become larger than one at larger x , termed as the anti-shadowing region. The difference between the nuclear PDF and proton PDF belongs to the category of “cold nuclear matter” (CNM) effect, in contrary to the “hot nuclear matter” effect from the QGP medium. The CNM effect has to be included to correctly interpret the experimental data, though the current level on uncertainty on the nuclear PDF is still large.

4.1.3 Inclusive program versus Monte-Carlo event generator

In the course of my study, I have tried using both the inclusive cross-section program as well as a Monte-Carlo event generator to initialize the heavy quark production. The inclusive program directly applies the factorization theorem and computes the inclusive spectra of heavy quark / hadron production spectrum; while the event generator used the probabilistic picture of the DGLAP evolution to build an exclusive final state.

Initialize from inclusive cross-section program We use FONLL (Fixed-Order-Next-to-Leading-Log) to generate the inclusive production cross-section of heavy flavor at the partonic level [124]. The FONLL program is a combination of the fixed order (NLO) massive matrix-elements and a massless resummation program. It computes the single inclusive differential cross-section of heavy quark / hadron production $d^2\sigma/dydp_T$. Using $d^2\sigma/dydp_T$, heavy quark’s initial momentum is sample.

It has the advantage of being a first principal calculation when applied to proton-proton collisions, but the main disadvantage is the lack of an exclusive partonic final state. This causes several problems,

1. Limit the study to open-heavy flavor. For full jet study, one needs the exclusive partonic final state. For quarkonium study, the momentum correlations among the Q - \bar{Q} pairs are important.
2. We cannot build a space-time picture of the parton shower to implement medium modifications to parton evolution. Therefore, in this initialization routine, we have always assumed the vacuum-like evolution has already finished at time $\tau = 0^+$.

Initialize from Monte-Carlo event generator We used Pythia (version 8.235) as the hard parton generator [125, 126]. Pythia implements the leading order (LO) matrix-elements for hard QCD processes, including LO production of heavy flavor particles, $g + g \rightarrow Q + \bar{Q}$ and $q + \bar{q} \rightarrow Q + \bar{Q}$. A parton shower include initial state radiation (ISR) and final state radiation (FSR) is generated around the hard vertex. At high energy, the LO production of heavy flavor is only a fraction of the total heavy flavor cross-section, the rest of them are created actually in the parton showers via the so-called “gluon splitting” and “flavor creation” processes. The former corresponds to a situation where the heavy flavor pair comes from a final state gluon splitting; and the latter produces the pair in initial state gluon splitting and is put-on shell by the hard scattering. These contributions also mimic certain pair correlations with non back-to-back angular correlations.

This initialization method is not a first principal approach. Also generation of full parton shower at the LHC energy can be slow, but the benefits are enormous,

- Though the parton shower in Pythia is evolved as a function of virtuality Q^2 , an approximate space-time picture can be reconstructed by defining the formation time for each branching $2x(1-x)E/Q^2$. Then, it is easy to determine which splitting happened inside the medium and receives medium modifications.
- Allow an initialization of full jet evolution and the study of quarkonium transport.

A comparison of proton-proton baseline and CNM effect We checked whether the pythia event generator products similar proton-proton baseline compared to the first principle approach FONLL. In the upper plot of figure 4.3, we compare the p_T differential cross-section of $p + p \rightarrow c$ from FONLL (lines) and Pythia simulations (symbols), and for Pb+Pb collision (red) and p+p collision (blue) at the LHC energy $\sqrt{s} = 5.02$ TeV.

For proton-proton collisions, we use the CT10 parton distribution function [127]. The nuclear PDF uses the EPS09 parametrization [128].

Though the absolute value of the cross-sections between FONLL and Pythia are different, the interested observables are always ratios between nuclear collisions and the proton-proton baseline where normalization cancels, or other dimensional-less observables such as the momentum-space anisotropy of heavy meson. Therefore, we focus more on the shape of the spectra between the two calculation, which agree very well. The ratio of initial charm spectra of Pb+Pb collisions and p+p collisions estimates the magnitude of the cold-nuclear matter effect on the nuclear modification factor R_{AA} (without the hot QGP effect). FONLL and Pythia simulation predict consistent modulation: the initial production AA spectra of charm quark at low- p_T is suppressed compared to the pp spectra, due to the shadowing effect of the small- x gluon. At higher p_T , the ratio increase and slightly shoots over unity, because partons from the anti-shadowing contribute more at larger- x .

4.2 Matching vacuum and medium-induced showers

4.2.1 A separate treatment of different phase-space

The fate of vacuum-like showers in the hot-medium is complicated and there has not been a lot of phenomenological studies [Caucal:2018tlu, 114, 117, 118]. The prescription that we build in this section is by no means exact, but follow the reasoning from a recent work [117]. The general idea is to identify different regions of phase-space of radiation, and apply different computation (DGLAP / transport) to different regions based on how much medium-modifications it would have received.

Considering a vacuum splitting of a hard parton that enters the medium at $z = 0$. The vacuum splitting has formation time $\tau_f \sim 2x(1-x)E/k_\perp^2$. It is very likely that the radiated gluon (or the quark) interacts with one or more scattering centers (labeled by “i”) in the medium at time t_i . Whether these interactions contribute coherently to the “vacuum-like” splitting follows the same argument as before. Scatterings that are well separated from the formation processes $\tau_f \ll t_i$ are treated as independently, and it only broadens the transverse momentum without changing the probability of the process. For $t_i \lesssim \tau_f$, the branching probability of the vacuum-like radiation also gets modified, in addition to broadening. Now classifying the radiations

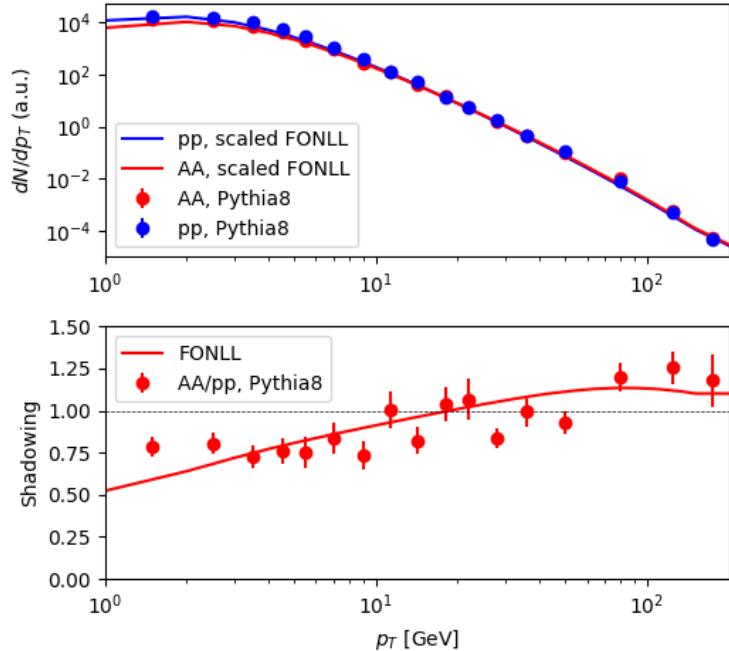


Figure 4.3 Top plot: a comparison of D -meson production in proton-proton collisions (blue) and in Pb-Pb collisions (red) with cold nuclear matter effect only. FONLL calculations are shown in lines and Pythia8 simulations are shown in symbols. Bottom plot: the ratio between the production in Pb-Pb collision (cold nuclear matter effect only) to the proton-proton baseline shows the nuclear shadowing effect.

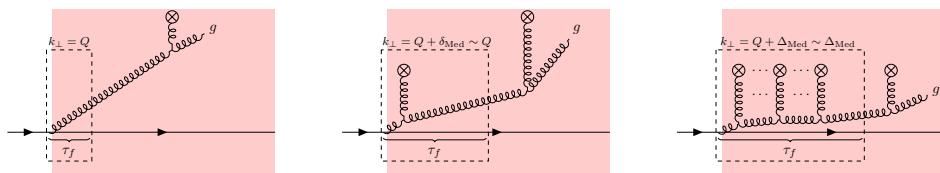


Figure 4.4 Demonstration of the medium corrections to vacuum-like radiation with different formation time. The energy of the gluon is hold fixed, while the virtuality is decreasing from left to right.

using the average “number” of scatterings $N = \tau_f/\lambda$ (for the case of a static medium),

- For a branching with large virtuality (left of figure 4.4) so that $N \ll 1$ or equivalently $Q^2 \gg g^2 x(1-x)ET$. The chance for the medium modification the vacuum branching probability is negligible.
- Hold the energy of the radiation and decrease its virtuality (middle of figure 4.4) so that $N = \tau_f/\lambda \sim 1$ ($Q^2 \sim g^2 x(1-x)ET$). Now, there is an order one probability of scatterings within τ_f , but the transverse momentum of the gluon is still dominated by the initial virtuality. The probability for the branching should also be modified accordingly, for example, using the higher-twist formula that expanded in terms of $1/Q^2$.
- Further decrease the initial virtuality of the branching (right of figure 4.4) until $N = \gg 1$, the medium broadening to the branching eventually dominates over the the virtuality. And $Q^2 \sim g^2 \sqrt{x(1-x)ET^3}$. When this happens, the branching probability is heavily modified by the medium and should be replaced by a medium-induced splitting calculation.

Summarizing the two extreme regions: The DGLAP evolution is applied to the high-virtuality part of the shower $Q^2 \gg \alpha_s \omega T$ is not modified, while medium-induced calculations should be applied to the low-virtuality shower $Q^2 \sim \sqrt{\hat{q}\omega}$ (relation obtained in a static medium) via transport equations. It is therefore natural to use the comparison relation between the partons’s original virtuality Q^2 and the transverse momentum change contributed by medium broadening $\Delta k_\perp^2 = (\mathbf{k}_\perp(\tau = \tau_f) - \mathbf{k}_\perp(\tau = 0))^2$ to separate the medium-induced radiation and the vacuum-like radiation. The matching prescription is then to simply cut-out the vacuum branchings generated by Pythia in the region $\Delta k_\perp^2 \gtrsim Q^2$, the cut region is referred as the “vetoed” region in the literature [117]). For a dynamical and fluctuating medium, there is no simple relation as $\Delta k_\perp^2 \sim \sqrt{\hat{q}\omega}$ in the static medium, but the “preformed parton” technique can be used determined Δk_\perp^2 self-consistently for each vacuum branching (to be explained in the next paragraph). Also in a finite medium, certain vacuum-like branchings may have a long formation time that it forms outside of the medium, from the uncertainty principle, these branchings do not resolve the details of the medium and its branching probability will not be modified in our model. This separated treatment of different region of phase-space still depends on the detailed choice of the

separation scale, so in the future, it would be ideal to develop a unified theoretical treatment for both vacuum and medium-induced shower in the time evolution picture.

Focusing only on the vacuum-like radiation generated by heavy quarks, one traces back a heavy quark line in the Pythia event recorder to find all the gluons from its final state radiation (FSR) and the original four momentum of the heavy quark at initial production vertex. These FSR gluons are first treated as “unformed” by the transport models, and they are allowed to undergo elastic broadening with the medium. In this way, by the time these gluons reaches its formation time ($t - t_0 > \tau_f$), one knows both the initial virtuality and of the splitting Q^2 , as well as how much medium broadening is acquired Δk_\perp^2 . Then, applying for our previous approximation, vacuum-like branching with $\Delta k_\perp^2 < R_v Q^2$ is unmodified, but $\Delta k_\perp^2 > R_v Q^2$ ones are rejected because this contribution is already taken care by the medium-induced rate in the transport model. The order one R_v parameter is introduced to parametrize the uncertainty in this matching scale.

4.2.2 Visualizing the matching on the Lund diagram

The Lund diagram is a useful tool to visualize the phase-space for high energy parton splitting. There are many different choice of kinematic variables, but here we choose the vertical axis to be $Y = \ln(1/x) = \ln(E/\omega)$, and the horizontal axis to be $X = \ln(1/\theta^2) = \ln(\omega^2/k_\perp^2)$. Here x is the energy fraction carried by the daughter parton in a particular splitting, and θ is the daughter’s emission angle relative to the mother parton. This arrangement is inspired by the soft and collinear limit of the QCD splitting function (for example $q \rightarrow q + g$),

$$dP_{qg}^q \sim \frac{\alpha_s C_F}{\pi} \frac{dx}{x} \frac{d\theta^2}{\theta^2} = \frac{\alpha_s C_F}{\pi} d\ln \frac{1}{x} d\ln \frac{1}{\theta^2}. \quad (4.2)$$

Therefore, the probability distribution of a vacuum-like splitting vertex should be uniform, apart from the running coupling effect. The closer a point lies towards the origin, the higher its virtuality. The soft and collinear radiations reside at large X and Y . Also, constant-formation-time contours are simply straight lines $Y + X = \ln(E\tau_f/2)$.

On the left of figure 4.5, we show the phase space occupied by the vacuum branching without medium (left); on the right, it is medium-modified vacuum splitting (blue color map) and the medium induced radiation (red contour) from our simulation. The simulation first finds out charm quark

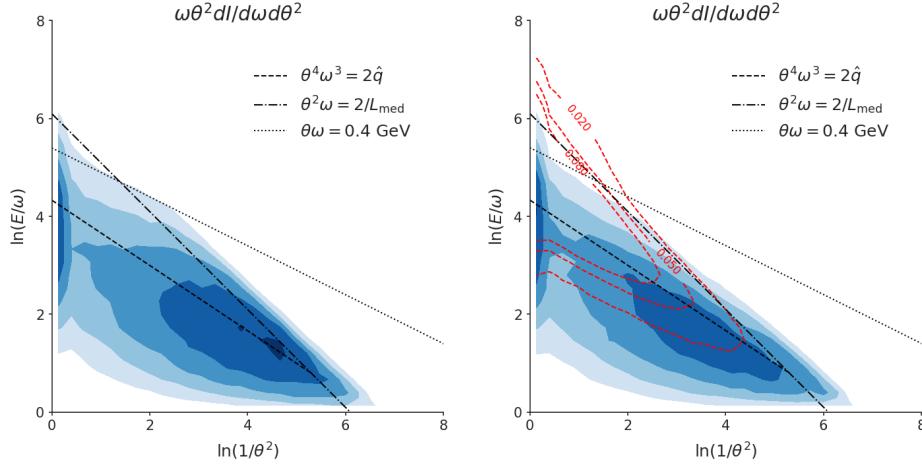


Figure 4.5 Plotting the gluon radiations from a charm quark on the Lund diagram. The gluon emission has an energy ω with angle θ with respect to the heavy quark. The blue heat map in the left plot shows the distribution of vacuum-like emissions without medium effects. The heat map in right left plot shows the distribution of vacuum-like emissions with medium effects; while the red contour stands for the medium induced emissions. Emissions on the black dashed lines have $k_\perp^2 = \sqrt{2\omega\hat{q}}$. Emissions on the dashed-dotted lines have a formation time equals to the medium path-length. Finally, the dotted lines is the non-perturbative cut-off in Pythia $k_\perp = 0.4 \text{ GeV}$.

with transverse momentum $90 < p_T < 110 \text{ GeV}$ at the production vertex in Pythia, and then propagate it and its vacuum radiated gluons in a static medium with $T = 0.3 \text{ GeV}$ with $\alpha_s = 0.3$ for a path length L . We see that without the medium effect, the vacuum radiations fills the region bounded by time-evolution limit $\tau_f < L$ (dash-dotted line) and the default non-perturbative bounds $k_\perp > 0.4 \text{ GeV}$ (dotted line) of Pythia. Inside the medium, the medium-induced radiations distributed around the line $\tau_f \hat{q} = k_\perp^2$ which is $\theta^4\omega^3 = 2\hat{q}$ (dashed line) in the soft limit. But this line is only an averaged estimation of the relation between k_\perp, ω and \hat{q} , the actually outcome of the simulation has huge fluctuation. The triangle area bounded by the line $\tau_f < L$ and the line $\theta^4\omega^3 = 2\hat{q}$ is where the vacuum-like radiation receives large modification from medium interactions. The rejection program introduced before suppress the vacuum-like radiation in this region compared to the case without a medium. Again, due to fluctuations, the triangle region is not an entirely vetoed as the one demonstrated in [117].

Concluding this section, the realm of the transport equation and the

DGLAP evolution is separated when the parton virtuality is comparable to the acquired transverse momentum broadening within the formation time. High virtuality evolution is approximated as unmodified, while low virtuality evolution is terminated and replaced by the medium-induce processes via the transport evolution. Using the Lund diagram to visualize the simulation, medium-induced and vacuum branchings occupy relatively separated region of the phase-space, though smeared by a large fluctuation. This procedure is, of course, only viable if we initialize the simulation with parton shower event generator. We are not able to do such a separation using heavy quark spectra obtained from FONLL.

4.3 Particles coupled to an evolving medium

The coupling between hydrodynamics and hard parton transport often require a switching of different reference frames, as velocity of the medium local-rest-frame relative to the lab frame is function of space-time.

For diffusion dynamics The diffusion equations are most easily written in the local-rest-frame of the medium. Given a particle's four momentum in the lab frame (p_L^μ), one first boost it into the medium local-rest-frame (p_M^μ),

$$p_M^\mu = L_\nu^\mu(\vec{\beta}) p_L^\nu \quad (4.3)$$

$$L_\nu^\mu = \begin{bmatrix} \gamma & -\gamma\vec{\beta} \\ -\gamma\vec{\beta} & \mathbb{1} + \frac{\gamma^2}{\gamma+1}\vec{\beta}\vec{\beta} \end{bmatrix} \quad (4.4)$$

where $\vec{\beta}$ is the velocity of the fluid cell relative to the lab frame, and L_ν^μ is the Lorentz transformation. One needs to be careful with that the time step in the fluid rest frame Δt_M is different from the one in the lab frame Δt_L . Consider the particle trajectory Δx_L^μ within Δt_L observed in the lab frame and boost it into the medium frame,

$$\Delta x_L^\mu = \frac{p_L^\mu}{E_L} \Delta t_L \xrightarrow{\text{boost}} \Delta x_M^\mu = \frac{L_\nu^\mu(\mathbf{v}_M) p_L^\nu}{E_L} \Delta t_L = \frac{p_M^\mu}{E_L} \Delta t_L \quad (4.5)$$

Now compare the time-component of the equation, one get the time step in the medium frame is related to the lab frame step by the ratio between the energy of the particle in the two reference frames,

$$\Delta t_M = \frac{E_M}{E_L} \Delta t_L \quad (4.6)$$

Once the momentum is updated in the medium frame to become p'_M , it is boosted back to the lab frame,

$$x'^\mu = x^\mu + \frac{p'_L}{E_L} \Delta t_L \quad (4.7)$$

$$p'_L = L_\nu^\mu (-\vec{\beta}) p_M^\nu \quad (4.8)$$

where we have chosen to update position before the update of the momentum.

The choice of Δt_L is also tricky. A most straightforward uniform time step for all the particles is not the optimal choice. This is because that relativistic hydrodynamics for heavy-ion collision is often solved in the (τ, x, y, η_s) coordinates, and the hydrodynamic field is propagated from one constant proper time $\tau = \sqrt{t^2 - z^2}$ to the next. There are two consequences if we choose the same Δt_L for all particles:

1. Different particles will be at different proper times τ at a constant t . It requires the program to load the entire hydrodynamic temperature and velocity history into the memory, which can be a potential problem for 3+1 D hydro simulation (the memory consumption for boost-invariant hydrodynamics is not critical).
2. The time step in medium-rest-frame for particles at large space-time rapidity would be too small.

For these practical reasons, we choose to propagate particles with a constant proper-time step $\Delta\tau$. As a result, the time step in the lab frame is different for each particle, depending on its location and momentum, and is solved by,

$$\Delta\tau = \sqrt{(t + \Delta t_L)^2 - (z + v_z \Delta t_L)^2} - \sqrt{t^2 - z^2}. \quad (4.9)$$

This is (keeping the positive solution),

$$\Delta t_L(p, x) = \frac{-(t - zv_z) + \sqrt{(t - zv_z)^2 - (1 - v_z^2)(\Delta\tau^2 + 2\sqrt{t^2 - z^2}\Delta\tau)}}{2(1 - v_z^2)} \quad (4.10)$$

This adaptive time step propagate a particle between constant proper-time hyper-surface, therefore only two steps of hydrodynamic information needs to be loaded into memory at a time. Also Δt_L becomes larger for forward/backward particles.

For matrix-element scattering The situation for matrix-element scatterings is more complicated. Because the initial state of scattering is straightforwardly sampled in the medium local-rest-frame, but the full final state is most efficiently sampled in the center-of-mass frame of the few-body collisions. The center-of-mass velocity relative to the local-rest-frame is,

$$\vec{\beta}_C = \frac{\sum_{i \in IS} \vec{p}_i}{\sum_{i \in IS} E_i} \quad (4.11)$$

where “IS” stands for the initial state.

1. For each hard parton, determine Δt_L with equation 4.10.
2. Boost the particle to the medium rest-frame and sample the scattering rate $\Delta t_M R$ channel, and then sample the medium parton(s) that forms the scattering initial state with the hard parton.
3. In the CoM frame of the initial state, sample the final state particles.
4. Boost back the final state particles to the medium rest frame.
5. Boost back to the lab frame.

4.4 Heavy-flavor hadronization and hadronic stage

At a temperature around T_c , light hadrons can be sampled from the hydrodynamics energy momentum tensor statistically. For hard partons that stay more off equilibrium, a more microscopic hadronization model is in need. The final hadronic system is also dense enough for the heavy hadron to interact. Though the hadronic interactions are not analyzed so extensively as the QGP interaction, studies have shown hadronic rescatterings contributes finite low- p_T v_2 of D-meson [129]. Therefore we also includes the afterburner stage for the heavy flavors.

4.4.1 The “sudden” approximation of hadronization

The hadronization implementation is described in [107]. It combines the fragmentation of heavy quark at high momentum and the recombination with medium partons into hadrons at low momentum. The hadronization is treated to be instantaneous on an isothermal hypersurface. This “sudden” approximation certainly has certain drawbacks. First, hadronization is a long distance process. In the rest frame of the heavy flavor, it takes time

scale $1/\Lambda_{QCD}$. With a large boost factor $E/M_{\text{hadron}} \sim E/M_{\text{heavy quark}}$, the formation time of the heavy hadron can be comparable to macroscopic length scales. For example, for a moderate $E = 10$ GeV charm quark $M = 1.3$ GeV, this time is estimated to be 8 fm/c, which is certainly not a sudden process considering the hydrodynamic stage only last for $O(10)$ fm/c. Second, an instantaneous recombination process breaks energy conservation and detailed balance. Toward a solution to all these problems, one may need to consider using a dynamical hadronization model [130].

Fragmentation In high energy electron-positron collision and proton-proton collision, high momentum heavy quark hadronizes through the fragmentation mechanism. The energetic heavy quark produces a bunch of hadrons with a heavy hadron that carries a certainty fraction of the origin quark energy $z = p_H/p_Q$. The probability distribution of z is known as the fragmentation function $D(z)$, and can be measured in, e.g., electron-positron collier. There are different parametrizations for $D(z)$ and the Peterson fragmentation function [131] used in the present study,

$$D(z) \propto \frac{1}{z(1 - \frac{1}{z} - \frac{\epsilon}{1-z})^2} \quad (4.12)$$

where ϵ is a parameter that scales as m_Q^{-2} ($\epsilon_c \approx 0.05$, $\epsilon_b \approx 0.006$).

Recombination It was known already in proton-proton collision that heavy quark can hadronize into mesons by the recombination with a light quark in the proton remnant [132]. In a heavy-ion collision, recombination mechanism can play an important role for low transverse momentum heavy flavors, given the abundance of the medium thermal partons. Early study in the nuclear collisions [119] assumes that the recombination probability can be computed from the wave function overlap between initial state partons and final state mesons or baryons, with the momentum of the medium parton integrated over the thermal distribution.

$$\frac{dP_M(p', p)}{dp'^3} = \int dk^3 n_{\bar{q}}(k) W_M(p, k) \delta^{(3)}(\vec{p}' - \vec{p} - \vec{k}), \quad (4.13)$$

$$\frac{dP_B(p', p)}{dp'^3} = \int dk_1^3 dk_2^3 n_{\bar{q}}(k_1) n_{\bar{q}}(k_2) W_B(p, k_1, k_2) \delta^{(3)}(\vec{p}' - \vec{p} - \vec{k}_1 - (\vec{k}_2)) \quad (4.14)$$

On the left are the differential probability for a heavy quark with momentum p to hadronize into a heavy meson (first line) or a heavy baryon (second line) with momentum p' through recombination. They are equal to an integration of light quark(s) / anti-quark momentum of the production of baryon / meson

Wigner function W times the thermal distribution function, subjected to three-momentum conservation. It is evident that the energy conservation is not imposed in the instantaneous $2 \rightarrow 1$ coalescence approach. The quark / anti-quark distribution function is the Fermi-Dirac one, neglecting chemical potential,

$$n = \frac{g_q V}{e^{\beta p \cdot u} + 1} \quad (4.15)$$

with u the fluid velocity and the p the four momentum of the light quark / anti-quark. g is the degeneracy of the quark, and V is a test volume that will eventually be canceled by the normalization factor in the Wigner function. As a remark, we have assumed in the transport model that medium partons are massless because the thermal masses are higher effects for energy loss; but for recombination into bound states near T_c , it is important to use non-perturbative constituent masses of light quarks $m_u = m_d = 300$ MeV and $m_s = 475$ MeV.

Regarding the meson wave-function, there has been efforts using Dirac equation and to obtain a more realistic wave-function for different state of heavy mesons. But the current model uses parametrized Gaussian wave-function for simplicity,

$$\phi_M(\vec{r}) = \left(\frac{1}{\pi \sigma^2} \right)^{3/4} e^{-\frac{r^2}{2\sigma^2}} \quad (4.16)$$

The σ s are related to the reduced mass of the two body system $\mu = m_1 m_2 / (m_1 + m_2)$ and the frequency of the two-body potential ω by $\sigma = 1/\sqrt{\mu\omega}$. These frequencies are estimated from the charge radius of different heavy mesons: 0.106 GeV for charmed hadron and 0.059 GeV for the bottom mesons. The Wigner function is defined in terms of the relative distance \vec{r} and relative momentum \vec{q} between the quark and anti-quark,

$$W_M(\vec{r}, q^2) = g_M \int d^3 \vec{a} e^{-i\vec{q} \cdot \vec{a}} \phi_M(\vec{r} + \vec{a}/2) \phi_M^*(\vec{r} - \vec{a}/2) \quad (4.17)$$

$$\vec{q} = \frac{E_2 \vec{p}_1 - E_1 \vec{p}_2}{E_1 + E_2}. \quad (4.18)$$

Averaging over the light quark's positions,

$$W_M(q^2) = \frac{g_M}{V} (2\sqrt{\pi}\sigma)^3 e^{-\sigma^2 q^2}, \quad (4.19)$$

which is the quantity needed in equation 4.13,

$$\frac{dP_M(p', p)}{dp'^3} = \int dk^3 \frac{g_q g_M}{e^{\beta p \cdot u} + 1} (2\sqrt{\pi}\sigma)^3 e^{-\sigma^2 q^2} \delta^{(3)}(\vec{p}' - \vec{p} - \vec{k}), \quad (4.20)$$

where the test volume in the distribution function has been canceled by the one in the Wigner function.

The same procedure applies to heavy baryon, with the three-body Wigner function in the Gaussian approximation as,

$$f_B^W(q_1^2, q_2^2) = \frac{Ng_B}{V^2} (2\sqrt{\pi\sigma_{1,2}\sigma_{12,3}})^6 e^{-q_{1,2}^2\sigma_{1,2}^2 - q_{12,3}^2\sigma_{12,3}^2}. \quad (4.21)$$

With the relative momenta defined as,

$$\vec{q}_{1,2} = \frac{E_2\vec{p}_1 - E_1\vec{p}_2}{E_1 + E_2} \quad (4.22)$$

$$\vec{q}_{12,3} = \frac{E_3(\vec{p}_1 + \vec{p}_2) - (E_1 + E_2)\vec{p}_3}{E_1 + E_2 + E_3} \quad (4.23)$$

And the σ related to the frequency and masses by,

$$\sigma_{1,2}^{-1} = \sqrt{\omega \frac{m_1 m_2}{m_1 + m_2}} \quad (4.24)$$

$$\sigma_{12,3}^{-1} = \sqrt{\omega \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}} \quad (4.25)$$

To synthesis these two competing mechanisms of hadronization, one first samples the recombination probability in equations 4.13 and 4.14 and determines whether the heavy quark coalesces with the medium partons. If not, its hadronization will be handled by the Pythia fragmentation routine with the Peterson fragmentation function.

4.4.2 Hadronic rescattering

Currently, the hadronic rescattering of charmed mesons with π and ρ mesons are included the UrQMD frame as the light hadrons. These cross-sections are obtained from [133]. Hadronic cross-section of the charmed baryons and bottom hadrons are not included.

One modification is made to the UrQMD heavy-flavor sector that the back reaction from heavy flavor mesons to light sector is turned-off. This is done by resetting the light scattering partner's four momentum back to its initial value. This is to the same level of approximation of the linearized transport equation in the QGP phase, and allows for an easy oversampling of the number of heavy flavor particles to obtain better statistics.

4.5 Benchmark calculation of observables

In the last section of this chapter, we provide a benchmark calculation of this open-heavy flavor simulation framework to experimental data, systematic calibration of model parameters and uncertainties will be discussed in the next two chapters.

4.5.1 Open heavy flavor observables

Experimentally, the ground states mesons $D^0, \bar{D}^0, D^\pm, B^\pm, D_s^\pm, B_s^\pm$ and the excited states $D^{*\pm}$ can be measured in the experiments. Their nuclear modification factor, momentum anisotropy has been measured at both LHC and RHIC. Currently, we focus on comparing to non-strange D and B mesons data. Though strange heavy meson D_s, B_s are also very interested as they contain the strangeness enhancement information, but the strangeness physics is not the main focus of this work.

The nuclear modification factor has already been introduced in the chapter 1. Here we summarize how the momentum anisotropy observables are computed. A list of the measurements and references can be find in table 4.1 and table 4.2.

Table 4.1 ALICE dataset

Observables	Centrality	Reference
D -meson v_2	30-50%	Acharya:2017qps
Event-engineered	30-50%	Grosa:2017zcz
D -meson v_2		
D -meson R_{AA}	0-10, 30-50, 50-80%	Acharya:2018hre

Table 4.2 CMS dataset

Observables	Centrality	Reference
D^0 -meson v_2	0-10, 10-30, 30-50%	Sirunyan:2017plt
D^0 -meson R_{AA}	0-10%, 0-100%	Sirunyan:2017xss
B^\pm -meson R_{AA}	0-100%	Sirunyan:2017oug

Momentum anisotropy Heavy flavors momentum anisotropy at high- p_T is thought to be the result of anisotropic energy loss, because hard partons

emitted in the short axis direction losses less energy than those emitted from the long axis direction on average. At low momentum, the momentum anisotropy has a flow origin that heavy quark interacts so frequently with the medium and tends to catch up with the flow velocity of the medium. Both mechanisms produce v_2 relatively the common reference of bulk geometry / bulk flow. The p_T differential v_2 is usually measured in two-particle correlation approach,

$$v_n\{2\}(p_T) = \frac{\Re e \langle d_n\{2\} \rangle}{\langle c_n\{2\} \rangle}. \quad (4.26)$$

c_n is the event-wise two particle correlation of N reference particles (REF, the bulk medium) within a certain kinematic range,

$$c_n = \frac{|Q_n|^2 - N}{N(N-1)}, \quad (4.27)$$

$$Q_n = \sum_{i=1}^N e^{in\phi}, \quad (4.28)$$

and the event average ($\langle \cdots \rangle$) is weighted by $N(N-1)$. d_n is the correlation between the M particles of interest (POI, in this case the heavy flavors) and the N reference particles,

$$d_n = \frac{q_n Q_n^* - m}{MN - m}, \quad (4.29)$$

$$q_n = \sum_{j=1}^M e^{jn\phi} \quad (4.30)$$

m is the number of POI that is also counted as REF to subtract auto-correlations. The event average is weighted by the number of pairs $MN - m$.

Event-shape engineering on heavy-flavor v_2 Event-shape engineering is a more recent idea to look at the detailed response of the hard sector to the medium geometry. Experimentally, an ensemble of events belongs to a certain centrality class is further classified according to its “event shape”, measured by q_2 ,

$$q_2 = \frac{|Q_2|}{\sqrt{N}}. \quad (4.31)$$

Due to event-by-event geometry fluctuation, the event shape in the a given centrality class can be vary dramatically. The ALICE experiment then measures the D meson v_2 with events having the 20% largest q_2 and events with

the 60% smallest q_2 . They found a large separation between the resulting v_2 with biased selected events compared to the v_2 calculated from unbiased events. This measurement quantifies the response of hard probe to the event geometry fluctuation while controlling multiplicity.

4.5.2 A first comparison to data

We do not intend optimize all the parameters in the model in this first comparison to data, but uses reasonable guess of the parameters to understand the model. The TRENTo parameters and the hydrodynamic transport coefficients are obtained from the high likelihood parameters in [12]. The heavy quark flavor starts to lose energy from 0.6 fm/c, and the matching condition between the vacuum-like radiation and the medium-induced radiation is $\Delta k_\perp^2 = R_v Q^2$ with $R_v = 1$. We used only leading order contribution from the weakly coupled theory, and tried both fixed coupling and running coupling. The default switching scale between a large- Q scattering small- Q is $Q_{\text{cut}}^2 = 4m_D^2$.

Fixed coupling First, we compute with fixed coupling constant. It should be understood as an effective in-medium coupling for both elastic and radiative processes. In figure 4.6, we present the results (lines and bands) with data points measured at $\sqrt{s_{\text{NN}}}s = 5.02$ TeV for D mesons (symbol with errorbars and boxes). Different line shapes corresponds to different coupling $\alpha = 0.2$ (dashed), 0.3 (solid), and 0.4 (dash-dotted). The types of observables are shown within each subplots, indicating the experiment collaboration, the collision system and the centrality.

Looking at the experimental measurements, R_{AA} increases with the centrality classes and displays a minimum around $8 < p_T < 10$ GeV. In the high- p_T end, the R_{AA} increases towards the baseline around one. This increase is slow, noticing the p_T is plotted on a log scale. In the low- p_T end, the R_{AA} quickly rises. There are many reasons for this, for example, the feeding from higher- p_T particles due to energy loss; the feeding from low- p_T particles that are pushed outward by the strong medium radial flow. In addition, the recombination hadronization mechanism also plays a part, as the D meson is gaining momentum (on average) in the recombination process. Based on the comparison to R_{AA} , a phenomenological value for a fixed α_s is around 0.3–0.4. However, such values cannot explain the large momentum anisotropy in mid-central collisions, e.g. centrality 30–50%. This is known as the D meson R_{AA} – v_2 puzzle, which also appears for leading light hadrons. There has been different solutions to this problem, such as the proposed

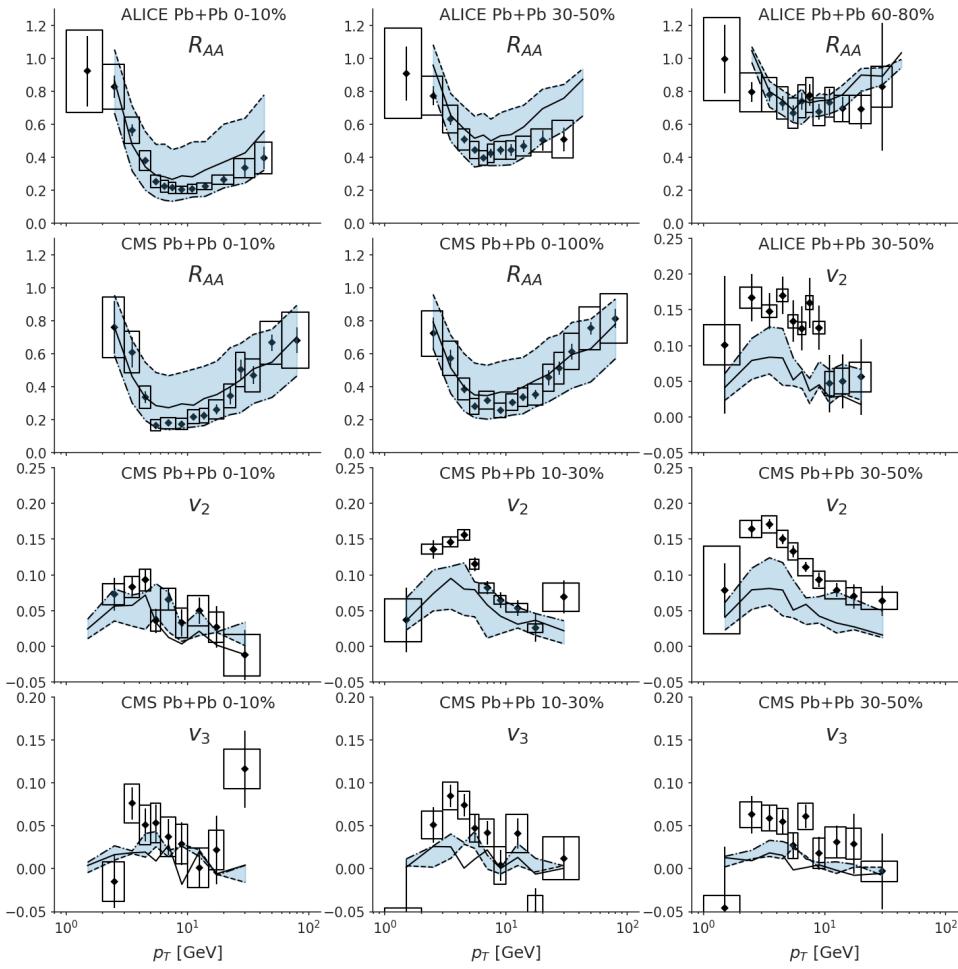


Figure 4.6 Benchmark results using fixed coupling constant $\alpha_s = 0.2$ (dashed), 0.3 (solid), and 0.4 (dash-dotted). The blue bands fill between the results using $\alpha_s = 0.2$ and 0.4. They are compared to the experimental data (black symbols) obtained by the ALICE Collaboration [134, 135] and the CMS Collaboration [136, 137].

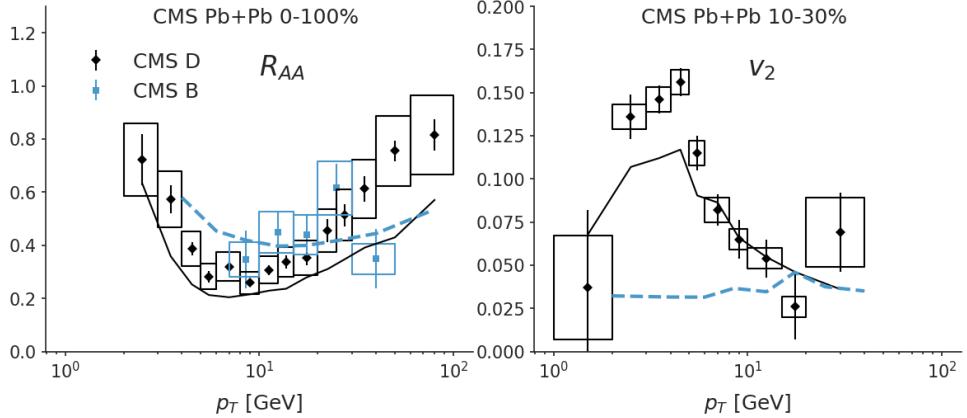


Figure 4.7 Demonstrating the mass dependence of the observables using $\alpha_s = 0.4$. The D meson and B meson results are labeled by color black and blue respectively. Left plot: R_{AA} for 0-100% centrality. Right plot: v_2 for 10-30% centrality.

sudden increase of the interaction strength near T_c , fine tuning the general temperature-momentum dependence of the transport coefficients, etc [138–140]. In the next two chapters, we will see if this discrepancy can be compensated by a fine tuning of parameters in the current model. A non-zero v_3 of D meson is an evidence of heavy-flavor coupling to the detailed event-by-event nuclear geometry fluctuation. The calculation of v_3 is systematically below the data, despite the large statistical and systematic uncertainty,

In figure ??, we compared the calculation with $\alpha_s = 0.4$ for charmed meson R_{AA}^D and bottom meson R_{AA}^B at 0 – 100% centrality and D meson and B meson flow at 10 – 30% centrality. The mass effect of bottom quark is much stronger than charm quark, therefore, R_{AA}^B at intermediate p_T is higher than R_{AA}^D . At very high p_T , the “Dead-Cone” of bottom quark also becomes insignificant, and the B and D meson R_{AA} converge. Unlike the sudden increase of v_2^D at low p_T , v_2^B is always small, meaning that the bottom quark does not catch up the medium flow as the charm does and remains far from equilibrium.

Running coupling Moving to a running coupling constant, the uncertainty of the in-medium coupling strength is transferred to the uncertainty of the medium scale in the running α_s ,

$$\alpha_s(Q) = \frac{2\pi}{9} \frac{1}{\ln(\max\{Q, \mu\pi T\}/\Lambda)}. \quad (4.32)$$

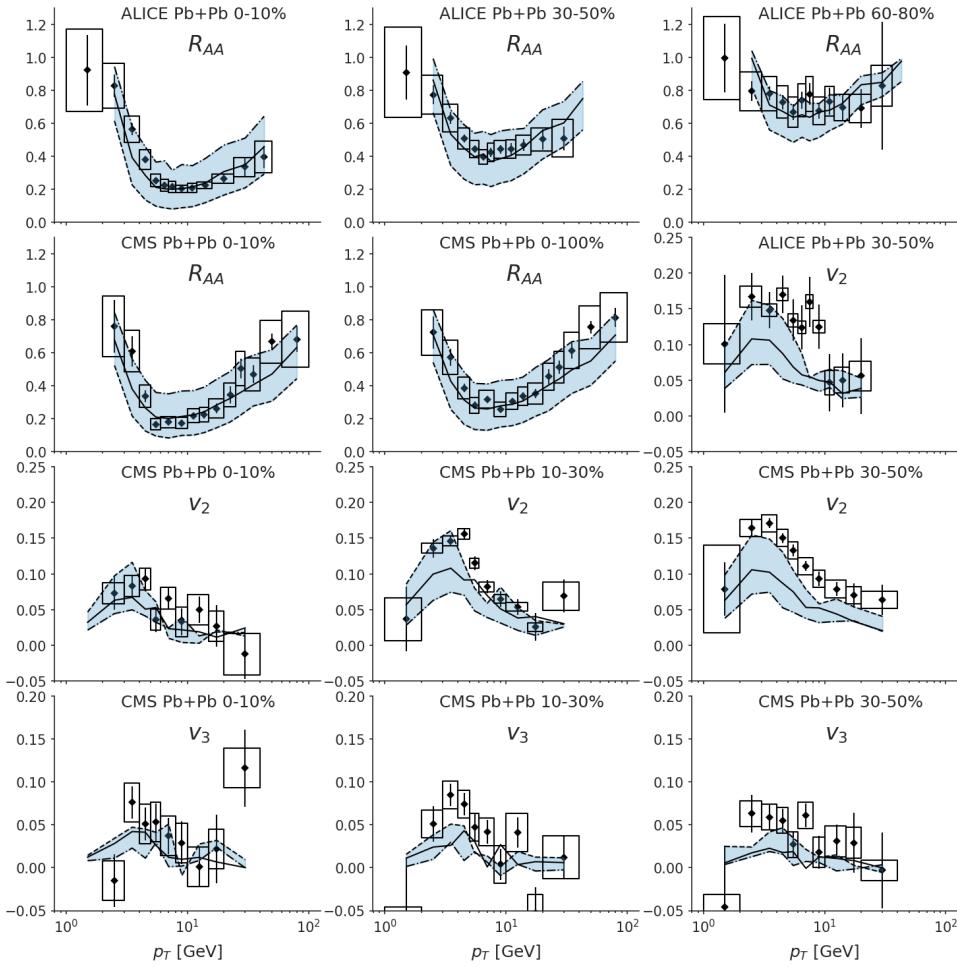


Figure 4.8 Benchmark results using running coupling constant. The medium scale that stops the low- Q running is chosen at $Q_{\text{med}} = \mu\pi T = \pi T$ (dashed), $2\pi T$ (solid), and $4\pi T$ (dash-dotted). They are compared to the experimental data (black symbols) obtained by the ALICE Collaboration and the CMS Collaboration.

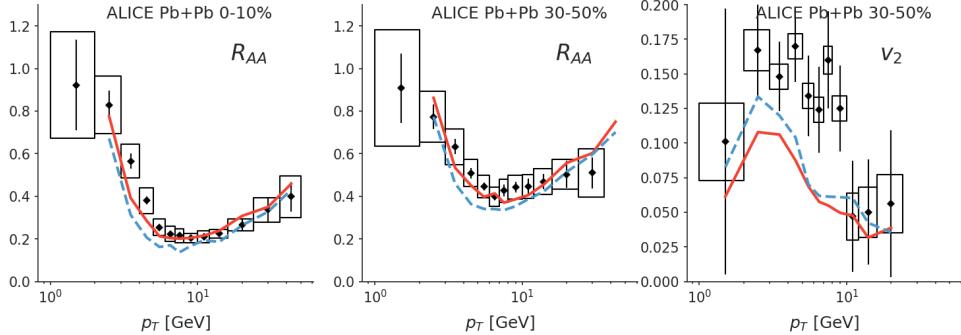


Figure 4.9 Effect of changing the switch scale between small- Q diffusion modeling and large- Q scattering modeling. $\mu = 2$ is used. The red solid lines used a switching scale at $Q_{\text{switch}}^2 = 4m_D^2$, and the blue dashed lines uses $16m_D^2$.

Due to the running, heavy quark radiation at high energy will be reduced compared to low energy and the interaction strength with the medium is enhanced at low temperature relative to high temperature.

In the comparison in figure 4.8, we choose $\mu = 1, 2, 4$, terminating the low- Q running of α_s at $Q = \pi T$ (dashed), $2\pi T$ (solid), $4\pi T$ (dash-dotted). We use πT as a natural unit because it is the typical thermal scale in the finite-temperature field theory calculations. Given that this entire heavy-flavor coupled-to hydrodynamic model is only an approximation, one should not think of the appearance of π so seriously. The $\mu = 2\pi T$ choice explains the nuclear modification factor for all centralities very well, but underestimates v_2 by 50%. The $\mu = \pi T$ case achieves a better agreement with v_n , but R_{AA} is systematically off. Therefore, going from fixed coupling to running coupling, the v_2 puzzle still exists.

Switching scale dependence By construction, the energy loss should be insensitive to the switching scale between the small- Q diffusion and the large- Q scattering in the high energy, weakly coupled limit. We check if this argument holds for phenomenology application. In figure 4.9, in addition to the default $Q_{\text{cut}}^2 = 4m_D^2$ (red solid lines), we also use $Q_{\text{cut}}^2 = 16m_D^2$ (blue dashed lines) to model more probe-medium interaction by diffusion than scattering. We found that the effect on high- p_T observable is small. Because the high- p_T dynamics is dominated by the radiation energy loss, whose Q_{cut} is indeed small as checked in chapter 3. Larger differences of R_{AA} and v_2 is observed at low- p_T . One reason for this is that the Q_{cut} independence argument obtained for high energy partons does not work very well for low velocity partons. Another reason is that despite the scattering dynamics and

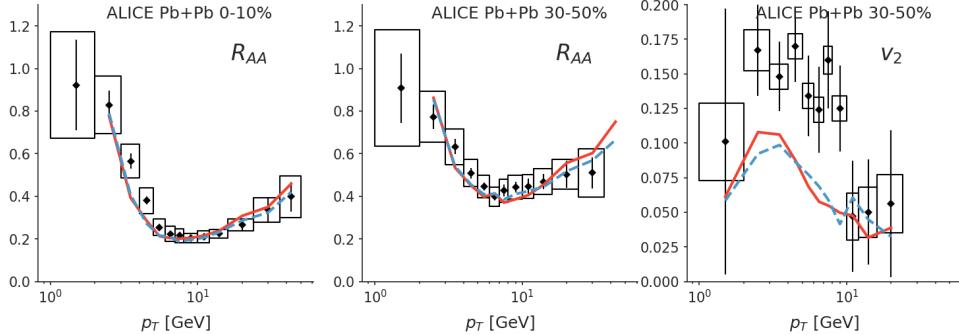


Figure 4.10 Effect of changing the matching scale parameter R_v ($\Delta k_\perp^2 = R_v Q^2$) between the vacuum-like shower and the medium-induced shower. $\mu = 2$ is used. The red solid lines use $R_v = 1$, while the blue dashed lines use $R_v = 1000$, which left the vacuum-like shower largely unmodified.

the diffusion dynamics has a matched diffusion constant (second moment of the momentum transfer), they are differed in all other momentum higher moment, in particular the drag (first moment). Remember that the drag coefficient in the diffusion dynamics is not a direct input from the weakly coupled theory, but is determined by the Einstein relation. The Einstein relation only guarantees that the diffusion dynamics evolves the system to the same equilibrium as the scattering dynamics, but the non-equilibrium path it takes can be very different from the scattering dynamics.

This Q_{cut} dependence may be bad at first sight, but one knows that the weakly coupled scattering picture does not necessarily work for the phenomenological coupling regime ($g \sim 2$), while the diffusion dynamics can be extended to strongly coupled regime. The Q_{cut} actually parameters an important source of theoretical uncertainty in our modeling.

Vacuum / medium-induced radiation matching scale dependence
As explained, there is a separation treatment of radiation that lives in different regions of phase-space on the lund-diagram. Accordingly, we need to subtract the vacuum radiation that overlapped with the medium-induced region in the Pythia event generator. In our earlier transport study of heavy flavor [75], this subtraction is not included, therefore, we would like to demonstrate the impact of this mistreatment here.

In figure 4.10, two calculations are shown. The red dashed lines stands the case where we removed vacuum-like radiations that satisfy $\Delta k_\perp^2 > Q^2$. The blue solid lines are calculations without this subtraction. The two calculations for R_{AA} only differs for $p_T \gtrsim 20$ GeV, because only high- p_T

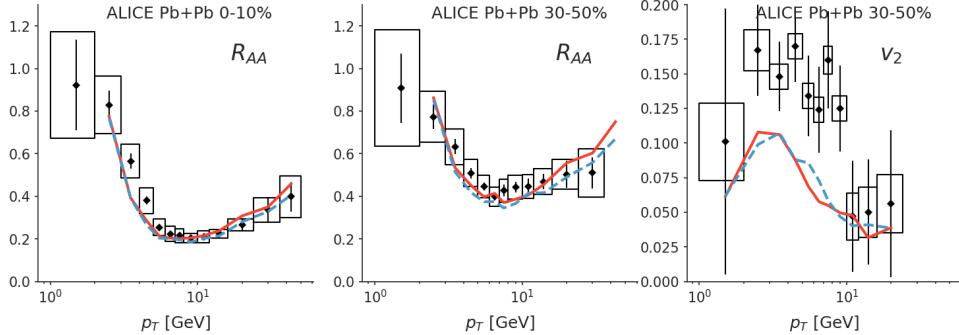


Figure 4.11 The impact of using “local rate” approximation. The red solid lines uses the default implementation; while the blue dashed line performs the rescatterings in an imaginary infinite box using locally defined temperatures to mimic the “local rate” approximation.

heavy quarks can undergo splittings that take long enough time to receive large medium corrections. Also the difference is large for central collisions than for peripheral collisions, because medium effect for the latter is weaker. No significant difference is observed for v_n .

Performance of the “local rate” approximation Finally, it is interesting to examine the effect of an “local rate” approximation of the radiative processes on the observables. It approximates the radiation probability in a medium with slowly varying temperature by the integration of radiation rates defined in an infinite static box with the local temperature at each point. One can also refers to it as the “adiabatic” approximation, because it really assumes the temperature variation is slow compared to the formation time.

We know this approximation can be broken by the fast expansion of the QGP fireball, and would like to quantify the impact. It is convenient to mimic the “local” approximation in our model, one can simply let the preformed-gluon rescattering procedure be done in an imaginary medium with the same temperature and flow velocity as those at the point of its production, instead of those in the evolving medium. The results comparison are shown in figure 4.11. The local approximation is good except at very high- p_T ($p_T > 30$ GeV).

5

Bayes parameter extraction of complex model

We have discussed the modeling details of the heavy flavor transport in the relativistic heavy-ion collisions, and have shown a first comparison to data with rather “naïve” guess of multiple parameters. Till now we have only vary a small subset of them to understand the model qualitatively. In this section, we introduce the advanced statistical tool known as the Bayesian analysis that can calibrate all parameters simultaneously to the experimental data. For the full details of such an analysis, we recommend the readers to this excellent dissertation of this subject [12] in the context of heavy-ion collisions.

To facilitate the discussion, I provide a statement of the problem for this chapter and a few notations and terminologies. We abstract the general task of a model-to-data comparison into the following form,

- A complex model M , with n input parameters organized as a n -dimensional vector \mathbf{p} .
- There is a prior belief on the reasonable range of each parameter, known as the prior probability distribution, and for short “Prior”.
- n experimental measurements are organized as an observation vector \mathbf{y}_{exp} of dimension m , with given statistical and systematic uncertainties $\delta\mathbf{y}_{\text{stat}}, \delta\mathbf{y}_{\text{sys}}$.
- The task is to infer the posterior probability distribution of p (Posterior), given the model M , the measurements $\delta\mathbf{y}_{\text{exp}} \pm \mathbf{y}$, and the Prior.

The analysis proceed as the following steps explained in each section.

5.1 Model evaluation on designed parameter sets

First, we need a fast evaluation of model M at any points in the considered region of parameter space.. This is done by sampling the high-dimensional input parameter space at N carefully designed points and then interpolating (next two sections). This N set of parameter vectors of length n forms a so-called design matrix \mathbf{D} ,

$$\mathbf{D}_{N \times n} = \begin{bmatrix} p_{11} & p_{12} & \cdots & p_{1n} \\ p_{21} & p_{22} & \cdots & p_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{N1} & p_{N2} & \cdots & p_{Nn} \end{bmatrix} \quad (5.1)$$

where the first index is the label of different parameter set, and the second index labels different parameters.

We used Latin-Hyper-Cube sampling method to design the location of these points in the parameter space. It generates a semi-random design subject to the following constraints:

- The marginalized distribution on any parameters is a uniform distribution. This is different from a grid design, where the marginalized distribution are spiky delta function on the grid points.
- The minimum distanced between any two points in the parameter space is maximized. This is different from a completely random design that points may form tight cluster or leave sparse regions.

Usually, for a well behaved model, the number of design points needed for a good interpolation increases linearly with the number of parameters n . This is in contrast a N exponential increasing with n in a grid design.

The actually model evaluation on these points are the time consuming part in this analysis. The outputs are organized into the observation matrix,

$$\mathbf{Y}_{N \times m} = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1m} \\ y_{21} & y_{22} & \cdots & y_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ y_{N1} & y_{N2} & \cdots & y_{Nm} \end{bmatrix} \quad (5.2)$$

where the first index is the label of different parameter set, and the second index labels different observables. The design matrix \mathbf{D} and the observations matrix \mathbf{Y} forms help to train a general interpolator to infer the calculated observables at any parameter set.

5.2 Data reduction

The model M is an n -dimensional vector to an m -dimensional vector mapping. One can certainly construct an array of independent m scalar mappings, and interpolate each of them. However, this naïve construction does not make use of the intrinsic correlations / structures that is already presented in the training data, and can be very inefficient for practice usage. Considering an observation with two values of R_{AA} and v_2 . Usually the larger the R_{AA} the model predicts, the smaller the v_2 , and thus an anti-correlation is expected. If one build interpolators for them independently, their uncertainties are also going to be independent, and the true covariance is omitted. However, if one interpolates the linearly combinations $aR_{AA} \pm bv_2$; then a wise choice of a, b can largely reduces the correlation between these two “newly” constructed observables.

The principal component analysis (PCA) is the systematic way to implement this idea. The original vectors of observables are transformed into the principal-component (PC) space, with each PC a specific linear combination of the original observables, so that the covariances between the newly defined observables (the PCs) vanish. Mathematically, this is the same as finding the singular value decomposition (SVD) of $\tilde{\mathbf{Y}}$. $\tilde{\mathbf{Y}}$ is the standardized observation matrix \mathbf{Y} ,

$$\tilde{y}_{ij} = \frac{y_{ij} - \mu_j}{\sigma_j} \quad (5.3)$$

with μ_j and σ_j the mean and the standard deviation of column j . Then the SVD proceeds as,

$$\tilde{\mathbf{Y}}_{N \times m} = \mathbf{U}_{N \times N} \boldsymbol{\Sigma}_{N \times m} \mathbf{V}_{m \times m}. \quad (5.4)$$

Here $\boldsymbol{\Sigma}$ only contains the variance of each PCs on its diagonal. The PCs are defined as the components after the V transformation.

$$z = \mathbf{V}y \quad (5.5)$$

It is evident that the covariance matrix of the z observables are diagonalized,

$$\text{Var}(z_i, z_j) = \frac{1}{N} V_{ii'} \tilde{Y}_{ki'} V_{jj'} \tilde{Y}_{kj'} = \frac{1}{N} V \tilde{Y}^T \tilde{Y} V^T = \frac{1}{N} \boldsymbol{\Sigma}. \quad (5.6)$$

So different PCs are orthogonalized. Another benefit is data reduction. Suppose the variance in $\boldsymbol{\Sigma}$ has been ordered from maximum to minimum. For data with pronounced structures, often the first few PCs take account

the majority of the data variance. Practically, a truncated set of PCs already gives a good representation of the original data, and this greatly reduces the computations for interpolating a large number of observables. Certainly, one can always go back from the PC space to the original space by the inverse transformation $y = V^{-1}z$.

5.3 Model emulator

With limited information on a finite number of design points contained in the matrices D and M , the original mapping is approximated by a model emulator (a surrogate model) using the Gaussian Process (GP). The Gaussian Process provides a non-parametric interpolation for scalar function with one or high dimensional input. We shall let the readers refer to [**Rasmussen:2006gp**] for the technical details and only summarize the basic of the Gaussian Process.

Gaussian Process Taking a uni-variate case as an example, given an array of input and an array of output, the common way to interpolate the data is, e.g., polynomial interpolation. However, polynomials only uses local information of the grid, and its performance can be sensitive to the error of the output (e.g. statistical fluctuation in the simulation). Moreover, it is hard to work with to a Latin-hypercube design because the design points are not arranged on a grid. In contrary, a GP does not make any assumption on the functional form of the interpolation, but infers the output at a certain input based on how the output at the present point correlates with those given outputs at other input points. Mathematically, one assumes that elements of the predicted output \mathbf{y}^* at input \mathbf{x}^* and the known outputs $\mathbf{y}_{\text{train}}$ at the training points $\mathbf{x}_{\text{train}}$ form a multi-variate normal distribution,

$$\begin{bmatrix} \mathbf{y}^* \\ \mathbf{y}_{\text{train}} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu^* \\ \mu_{\text{train}} \end{bmatrix}, \begin{bmatrix} \Sigma(\mathbf{x}^*, \mathbf{x}^*) & \Sigma(\mathbf{x}^*, \mathbf{x}_{\text{train}}) \\ \Sigma(\mathbf{x}_{\text{train}}, \mathbf{x}^*) & \Sigma(\mathbf{x}_{\text{train}}, \mathbf{x}_{\text{train}}) \end{bmatrix} \right) \quad (5.7)$$

μ^* and μ_{train} are the mean values and can be often set to zero after standardized the training data. The Σ s form the co-variance matrix, and each of them has the same shape of the outer product of its two arguments. Its matrix-element (the kernel function) are parametric, and one often takes a squared exponential form,

$$\Sigma_{ij} = k(x_i, x_j) = \sigma^2 \exp \left(-\frac{(x_i - x_j)^2}{2l^2} \right). \quad (5.8)$$

σ^2 is the auto correlation. The co-variance decays exponentially with the squared separation of the two input points. In such a way, points that are close in inputs will also be close in outputs, and points that are far apart are effectively uncorrelated.

Conditioning a Gaussian Process The outputs at training points are known. Therefore, the probability distribution of \mathbf{y}^* is obtained by conditioning the training outputs on their actually values,

$$\begin{aligned}\mathbf{y}^* \sim & \mathcal{N} \left(\Sigma(\mathbf{x}^*, \mathbf{x}_{\text{train}}) \Sigma^{-1}(\mathbf{x}_{\text{train}}, \mathbf{x}_{\text{train}}) \mathbf{y}_{\text{train}}, \right. \\ & \left. \Sigma(\mathbf{x}^*, \mathbf{x}^*) - \Sigma(\mathbf{x}^*, \mathbf{x}_{\text{train}}) \Sigma^{-1}(\mathbf{x}_{\text{train}}, \mathbf{x}_{\text{train}}) \Sigma(\mathbf{x}_{\text{train}}, \mathbf{x}^*) \right)\end{aligned}\quad (5.9)$$

Note that the conditional multivariate normal distribution is still a normal distribution, with modified mean and co-variance matrix. One can easily check that if the predicted input approaches one of the training input, the distribution of the output approaches an delta function (as the limit of a narrow Gaussian) at the training output.

Hyperparameters and training We have not discussed the parameters in the kernel function $k(x, x')$ too much yet. They are the auto-correlation σ^2 and the correlation length l . The squared exponential form is not the only possible kernel function, more sophisticated choices with more parameters are designed for varies problems. They are known as hyper-parameters (denoted as a vector θ), and should in principle, also be treated as unknown parameters in the calibration. But a common practice to reduce the complexity it to fix the hyper-parameters at a set of “optimal values” by minimize the loss function \mathcal{L} of the fitting,

$$\mathcal{L} = -\ln p(\mathbf{y}|\theta) = \frac{1}{2} \ln \det \Sigma(\theta) + \frac{1}{2} \mathbf{y}^T \Sigma(\theta)^{-1} \mathbf{y} + \frac{N}{2} \ln(2\pi) \quad (5.10)$$

where \mathbf{y} is the (PCA transformed) training data, and N is the number of training points. The minimization process is referred as “training” a Gaussian Process emulator.

Inference with uncertainty quantification Unlike the polynomial interpolation, a GP does not provide a single estimation of the output, but infers the probability distribution of the predicted outputs by giving both the mean and the co-variance matrix. This is a huge advantage of the Gaussian Process as it quantifies its own interpolation uncertainty.

Validation Though the training process includes certain penalty for over-fitting the data, whether the trained GP has over-fitting problem can only be checked by validation. A validation is done by performing the model calculation at novel points in the parameter space that is not “learned” by the GP, then comparing the trained GP’s prediction $y_i \pm \sigma_i$ to the model calculation $y_{\text{validate},i}$. If an emulator is trained to work properly, then the standardized deviation $(y_i - y_{\text{validate},i})/\sigma_i$ should follow approximately a standard normal distribution.

Multivariate inputs and outputs The GP formulation can be generalized to higher dimensional inputs easily by specifying a multidimensional kernel function. For high dimensional outputs, one first applies the PCA analysis introduced in the previous section and the build individual GPs for each of the first N_{PC} principal components that take most of the data’s variance.

5.4 Bayes’ theorem and Markov chain Monte Carlo

With the model emulator M (we are using the same symbol as the model, but one should always remember that the emulator is only a fast surrogate of the original model and comes with uncertainty), we apply the Bayes’ theorem, essence of the statistical analysis. The Bayes’ theorem is the quantitative way to update the knowledge of model parameters with empirical observations,

$$\text{Posterior}(\mathbf{p}|M, \mathbf{y}_{\text{exp}}) \propto \text{Likelihood}(\mathbf{y}_{\text{exp}}|M, \mathbf{p}) \times \text{Prior}(\mathbf{p}). \quad (5.11)$$

It states that the posterior probability distribution of parameters, given model and experimental measurements, is proportional to the likelihood to describe the experiments with the model using this set of parameters, times the prior belief of the distribution of the parameters. The likelihood is function is often assumed to be a multivariate Gaussian,

$$\begin{aligned} \text{Likelihood}(\mathbf{p}) &= (2\pi)^{-\frac{m}{2}} (\det |\Sigma|)^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} \Delta \mathbf{y}^T \Sigma^{-1} \Delta \mathbf{y} \right\}, \\ \Delta \mathbf{y} &= \mathbf{y}(\mathbf{p}) - \mathbf{y}_{\text{exp}} \end{aligned} \quad (5.12)$$

where the $\mathbf{y}(\mathbf{p})$ is the model emulators’ prediction at parameter point \mathbf{p} , m is the number of observables. The prior distribution is often a multi-dimensional uniform distribution within a reasonable range. The co-variance matrix contains various sources of uncertainties from both theory and experimental side.

A model dependent statement The posterior is always defined with a given model, and therefore even the extraction of theoretically well defined quantities can be affected by the use of different dynamical modeling. The ultimate solution is of course the improvement of model's physical accuracy. Or using a flexible model or models with different (but reasonable) assumptions to extract the same quantity and estimate the level of theoretical uncertainty.

The covariance matrix co-variance matrix is decomposed into different contributions,

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_{\text{stat}} + \boldsymbol{\Sigma}_{\text{sys}} + \boldsymbol{\Sigma}_{\text{emulator}} + \boldsymbol{\Sigma}_{\text{truncation}} + \boldsymbol{\Sigma}_{\text{model, sys}} \quad (5.14)$$

- The statistical co-variance takes the diagonal form, $\boldsymbol{\Sigma}_{\text{stat}} = \delta_{ij}\delta\mathbf{y}_{\text{stat},i}^2$. $\delta\mathbf{y}_{\text{stat},i}$ is the experimental statistical uncertainty.
- The experimental systematic uncertainties can be correlated for different observations, so generally its off-diagonal elements are non-zero,
- The emulator covaraince $\boldsymbol{\Sigma}_{\text{emulator}}$ is the prediction covariance of the GPs in the PC space and then transformed into the physical space.
- The truncation covaraince $\boldsymbol{\Sigma}_{\text{truncation}}$ take those less important principal components that are not being emulated by GPs into account. Its variance is first computed in the PC space and then transformed back to the physical space.
- Finally, $\boldsymbol{\Sigma}_{\text{model, sys}}$ stands for the model uncertainty. It is always present but is hard to quantify using the model itself. Therefore, the previous study [12] assign a variable model systematic parameters σ and this parameter will be treated as uncertainties in the calibration as well. The σ stands for a uniform model uncertainty fraction on each principal component, and is added to the emulator prediction covariance. The σ parameter is given an information prior distribution $P(\sigma) \propto \sigma^2 e^{-\sigma/0.05}$. Meaning an expectation of 15% model uncertainty. The exact origin of this model uncertainty is unknown, but it plays a role as a “regulator” in the fitting process to prevent model trying to explaining feature that can never be described better than the σ level precision.

Marginalize the posterior distribution The resultant posterior distribution is a function of n parameters. To answer what is the probability distribution of one parameter folded with uncertainty from other parameters,

one looks at the marginalized distribution with the other $n - 1$ parameters integrated out. This is done by a Markov chain Monte Carlo (MCMC) sampling of the posterior function and obtains an ensemble of n -dimensional walkers whose distribution thermalizes into the target posterior distribution function. The marginalized distribution is then the distribution of the projected ensemble onto one dimension. Similary, a marginalization of the joint distribution of two or more parameters can be obtained similarly.

6

Results

In this chapter, we apply the advanced statistical tools to the heavy-flavor transport model and extract the heavy quark transport coefficients. I would like to present this in a two step processes to show the improvements of the lastest extraction.

A list of experimental data

6.1 Lessons from earlier extractions of \hat{q}_Q

In an earlier publication [75], we used a linearized Boltzmann model with the coherence factor approach to implement the LPM effect. The heavy quark initial momentum dsitribution is obtained from the FONLL calculation. We have already commented on the advantages and disadvantages of these choices. Two different set of nuclear PDF *EPAPS* and *nCTEQ15* are used to represent the uncertainty from the cold nuclear matter effect in the \hat{q} extraction.

Regarding model parameters, the one parameter for the perturbative elastic and inelastic scatterings is controlled by $1/3 < \mu < 4$ in the running coupling. There is an additional pure diffusion process with a diffusion constant κ_{NP} parametrized to peak at low temperature and low energy, in order to mimic certain non-perturbative coupling between a low energy probe and the medium near T_c ,

$$\kappa_{NP} = T^3 \kappa_D \left(x_D + (1 - x_D) \frac{1 \text{ GeV}^2}{ET} \right). \quad (6.1)$$

The $0 < \kappa_D < 8$ parameter is the overall strength of the diffusion, and the $0 < x_D < 1$ controls the degree of energy-temperature dependence.

One can see that in the heavy quark limit $M \rightarrow \infty$, this parametrization becomes independent of mass. An additional parameter is the in-medium energy loss starting time τ_0 that is allowed to be tuned between $0.1 \text{ fm}/c$ to $1.0 \text{ fm}/c$ (before the onset of hydrodynamics). The reason is we lack a quantitative description of the production of color charge in the initial stages. This starting time is a simple approximation that interactions is only turned on after τ_0 when the color carries is assumed to approach a Boltzmann distribution.

The design of the four dimensional parameter space $(\tau_0, \mu, \kappa_D, x_D)$ has 80 design points. The computation is carried on the distributed computing system Open Science Grid [141, 142] using about a million CPU hours. The observables on which we calibrated are listed in tables 4.1 and 4.2. Including, p_T dependent D -meson nuclear modification factor R_{AA} and p_T dependent (event-shape-engineered) azimuthal anisotropy v_2 . CMS measurements of the B^\pm -meson R_{AA} is also included to constrain the mass dependence of the transport coefficients.

The prior and the posterior of the observables before and after the calibration is shown in figures 6.1 and 6.2. blue stands for using EPPS nuclear PDF and green stands for using the nCTEQnp nuclear PDF. We found that the model after the calibration provide a good description of R_{AA} and v_2 at the intermediate p_T of the ALICE experiments. But it does not reproduce the fast uprising shape of R_{AA} at high- p_T of the CMS experiment. In addition, the model seem to under estimate the high- p_T v_2 of the 30 – 50% centrality bin measured by CMS. The model is able to explain the correlation between the D-meson v_2 and the event-shape, though there are still large fluctuation in the data. The use of different nuclear PDFs has a negligible effect on v_2 , but does affect the R_{AA} at small and large p_T . Another thing worth noting that is that the D and B meson R_{AA} are described at the same time.

The inferred posterior probability distribution of the parameters is shown in the figure 6.3. The diagonal plots show single parameterized distributions, and the off-diagonal ones displays the two-parameter correlations. We split the results that use different nuclear PDFs into the upper (EPPS, green heat map and lines) and lower (nCTEQ15np, blue heat maps and lines) triangles. One notices that results from different nuclear PDF are consistent within the uncertainty; therefore, from now on I shall not stress on any differences between these two set of results, but combine them into a single distribution to fold in the PDF uncertainty. The favored parameters are $\mu \sim 0.6$ and $\kappa_D \sim 0.4$, indicating a large in-medium α_s and a small additional diffusion. The typical value of the α_s is, in fact, so large that let one worried about the

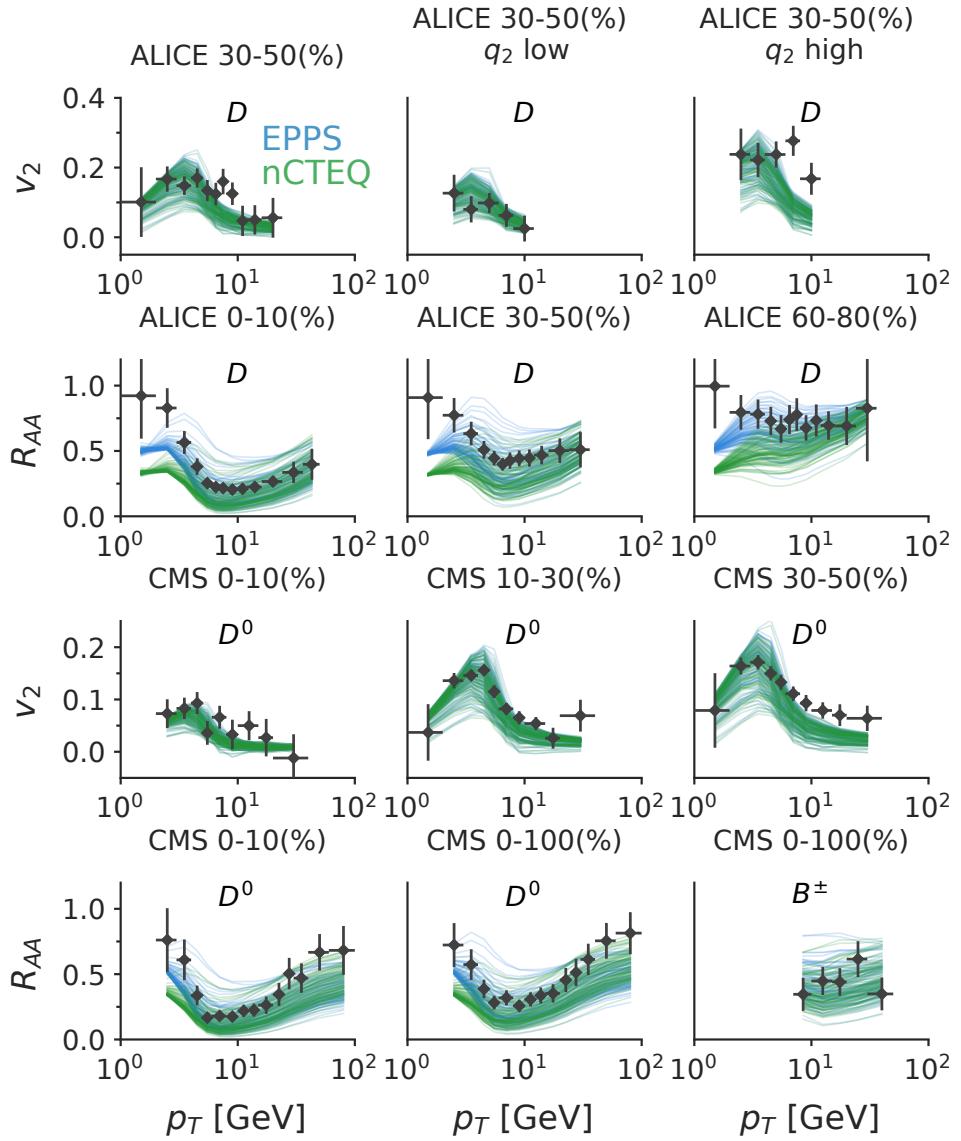


Figure 6.1 The prior distribution of observables compared to data. The colors labeled the use of EPPS (blue) and nCTEQ15np (green) nuclear PDF.

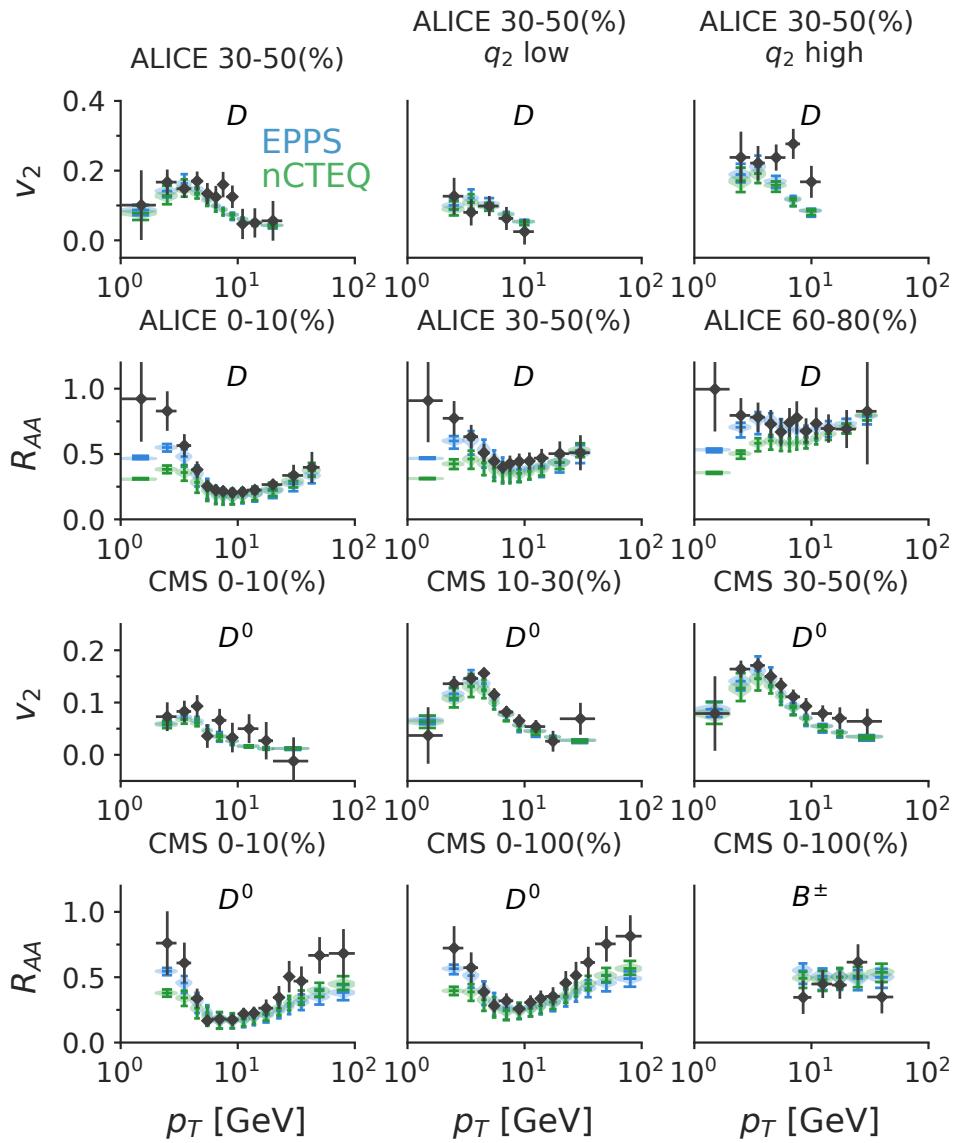


Figure 6.2 The 90% credible region of the posterior distribution of observables compared to data. The colors labeled the use of EPPS (blue) and nCTEQ15np (green) nuclear PDF.

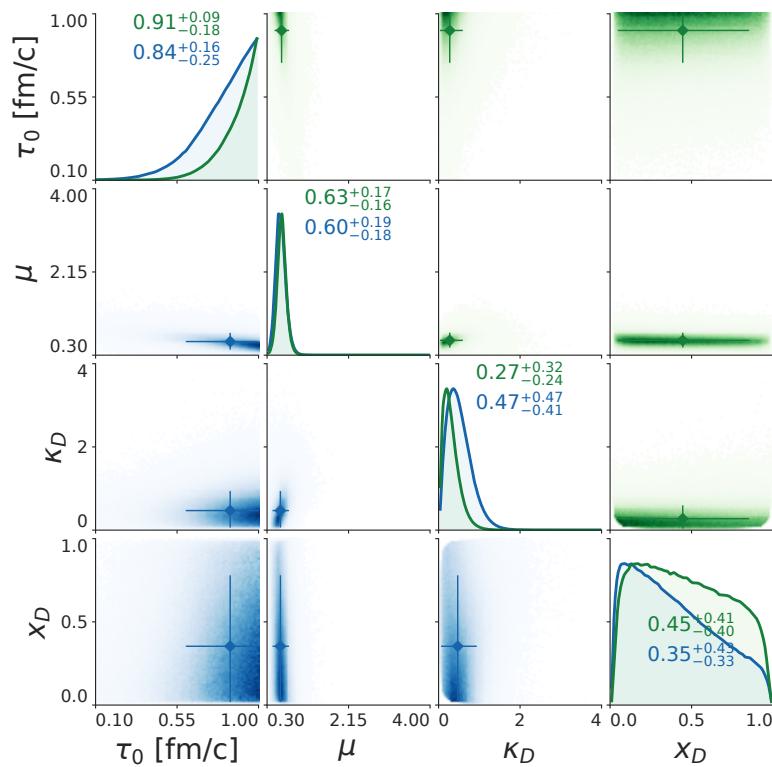


Figure 6.3 Posteriors of single-parameter distributions (diagonal plots) and two-parameter joint distributions (off-diagonal plots). The colors labeled the use of EPPS (blue) and nCTEQ15np (green) nuclear PDF.

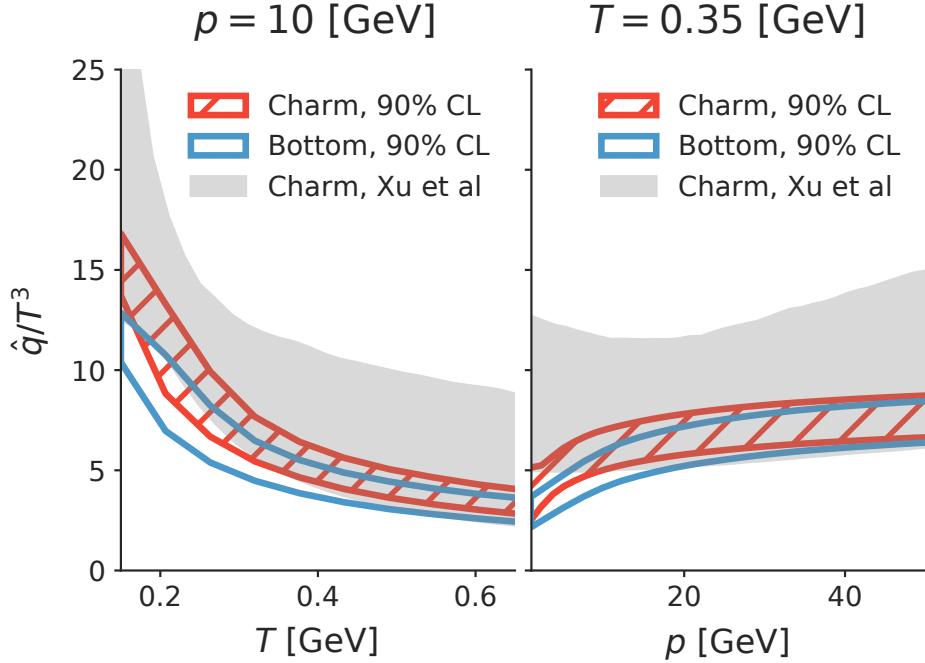


Figure 6.4 The 90% credible region of the heavy quark transverse momentum broadening parameter \hat{q} extracted using the model described in [75]. The charm quark results are shown in red, and bottom results in blue. The difference coming from using different nuclear PDF has been marginalized into the uncertainty bands. Left plot: the temperature dependence at $p = 10$ GeV. Right plot: the momentum dependence at $T = 0.35$ GeV.

use of weakly-coupled based approaches. For example, $\alpha_s(0.6\pi T)$ at $T = 300$ MeV is 0.67, corresponding to $g \approx 3$. And the screening mass $m_D \sim 3.6T$ is even larger than the average energy of the thermal partons $3T$. In the discussion of the next section, we will see that this problem can be slightly alleviated, once we use the improved implementation of the LPM effect and implement a separation of soft-modes into the diffusion constant, though g is still large.

Transport coefficients In this analysis, the heavy quark transport coefficient \hat{q} is computed from adding up the momentum broadening from both the scattering and the parametric diffusion,

$$\hat{q} = 2T^3 \kappa_D \left(x_D + (1 - x_D) \frac{\text{GeV}^2}{ET} \right) + \hat{q}_{\text{el}}. \quad (6.2)$$

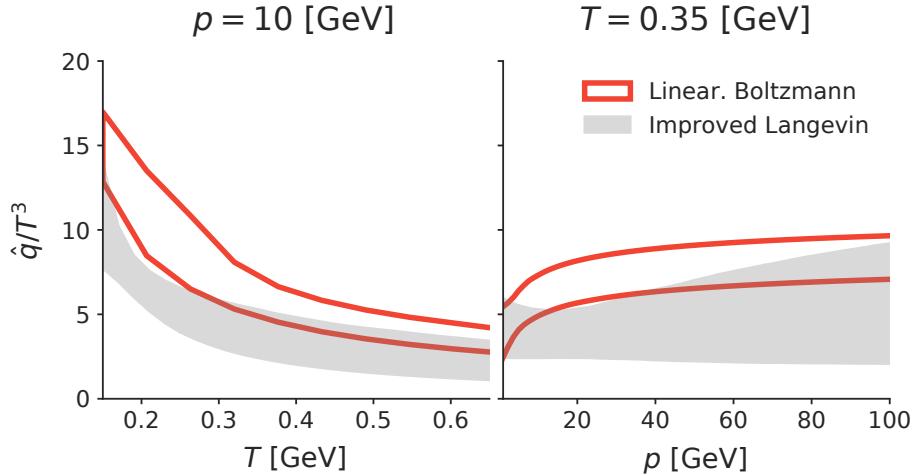


Figure 6.5 Comparing the 90% credible region of the charm \hat{q} using different models. The red regions use the model described in [75], while the shaded regions are obtained using the improved-Langevin model [107].

In a perturbative definition of the transport coefficients, the inelastic process does not contribute to heavy quark transport coefficient at leading order. In figure 6.4, the 90% credible region of \hat{q} is shown as a function of temperature at a fixed energy (left), and as function of energy at a fixed temperature (right). Results for charm (red) and bottom (blue) quarks are labeled by different colors. The mass difference only causes a small difference in \hat{q} .

Comparison to results from an improved-Langevin model The same transport coefficient is also extracted using the improved-Langevin model [107]. It includes a diffusion modeling of the elastic interaction, a high-twist single gluon emission rate, and a similar routine to implement multiple radiations. This model is then coupled to the same medium as the one used here and compared to the same set of observables as this work does. The resultant posterior (for charm quark only) is shown as the shaded region in figure 6.5. We see that the \hat{q} extracted using the two models only overlap at the boundary of the credible region. Their difference is comparable to the uncertainty band of either model, while both models provide a reasonable description of the data. This suggests the theoretical uncertainty that comes from the assumption between the probe and the medium is a significant one. The ability to tune a switching scale parameter in the new model intends to include this type of theoretical uncertainty.

6.2 Calibration using the improved transport model

Finally, we apply the improved model to the extraction of the heavy quark transport coefficients. As a summary of the improvements:

- A more sophisticated implementation of the LPM effect to reduce modeling uncertainty of the radiative process;
- An interpolation of the diffusion picture and the scattering picture to take into account modeling uncertainty.
- Separating the high-virtuality evolution and the low-virtuality transport equation at a medium scale.

Model parameters In the new analysis, we try to include as many theoretical uncertainty as possible, so we have much more parameters than the two previous studies. They are listed in table 6.1.

- The first parameter is again the energy loss starting time τ_i . In this analysis, we are comparing to data at two collision energies and the hydrodynamic starting time τ_0 varies from 1.2 fm/c to 0.6 fm/c. To account for this differences, we use the ratio $\xi = \tau_i/\tau_0$ as the single parameter for both energies. It means that after ξ fraction of the hydrodynamization time, the color density is assumed to be large enough to apply the linearized transport model.
- The second parameter is switching scale parameter $1.0 < c < 10.0$ in $Q_{\text{cut}}^2 = cm_D^2$. For a typical coupling $g \sim 2$, Q_{cut} is then varied from about $2T$ to $7T$.
- The third parameter $0 < R_v < 7$ controls the matching condition between the vacuum-like radiation and the medium-induce radiation $\Delta k_\perp^2 = R_v Q^2$. At $R_v = 0$, the vacuum-like radiation is completely forbidden once it interacts with the medium; for $R_v \gg 1$, the vacuum-like radiation is effectively unmodified.
- The $0.6 < \mu < 10$ parameter controls the in-medium strong coupling $\alpha_s(\max\{Q, \mu\pi T\})$.
- The rest of the six numbers K, a, b, p, q, γ parametrizes a correction to

Table 6.1 Prior range of parameters

Symbol	Description	Range
$\xi = \frac{\tau_0}{\tau_{\text{hydro}}}$	Energy loss starting time	(.1, .9)
$c = \frac{Q_{\text{cut}}^2}{m_D^2}$	Soft / hard switching scale	(.1, 10.)
R_v	Vacuum / Medium matching scale	(0, 7)
μ	Running α_s stops at $Q = \mu\pi T$	(.6, 10)
K	Magnitude of $\Delta\hat{q}/T^3$	(0, 15)
p	E -dependence of $\Delta\hat{q}/T^3$	(-2, 2)
a		(-1, 1)
q	T -dependence of $\Delta\hat{q}/T^3$	(-.5, 3)
b		(-.5, 3)
γ	$\Delta\hat{q}_L = (E/M)^\gamma \Delta\hat{q}_L$	(-1, 1)

the weakly coupled transport coefficient $\hat{q} + \Delta\hat{q}$, $\hat{q}_L + \Delta\hat{q}_L$,

$$\Delta\hat{q} = \frac{KT^3}{\left[1 + \left(a\frac{T}{T_c}\right)^p\right] \left[1 + \left(b\frac{E}{T}\right)^q\right]}, \quad (6.3)$$

$$\Delta\hat{q}_L = \left(\frac{E}{M}\right)^\gamma \frac{\Delta\hat{q}}{2} \quad (6.4)$$

$0 < K < 15$ is the overall magnitude of the correction. The deviation from the T^3 dependence and the energy dependence are parametrized using two dimensionless combinations T/T_c , and E/T . The γ parameter varied from -1 to 1 allows the correction to be anisotropic. Note that such a construction goes back to an isotropic diffusion when velocity approaches zero ($E \rightarrow M$).

Design and prior We chose to give $\ln c$, $\ln R_v$, $\ln \mu$, $\ln a$ and $\ln b$ a uniform design and a uniform prior. Therefore, the original parameter will have a non-uniform design and prior distribution. The reason is that these parameters either causes a logarithmic slow change in the model and its prior uncertainty is large that it is allowed vary by orders of magnitude. For example, the μ parameter enters the logarithmic running of α_s and we can rewrite the maximum possible α_s as,

$$\alpha_{s,\max}(T) = \frac{2\pi}{9} \frac{1}{\ln(\mu) + \ln(\pi T/\Lambda_{\text{QCD}})} \quad (6.5)$$

Therefore, we assign a uniform prior to $\ln(\mu)$ so that α_s also varies notably within the prior range. For the c and R_v parameter, we have seen in the

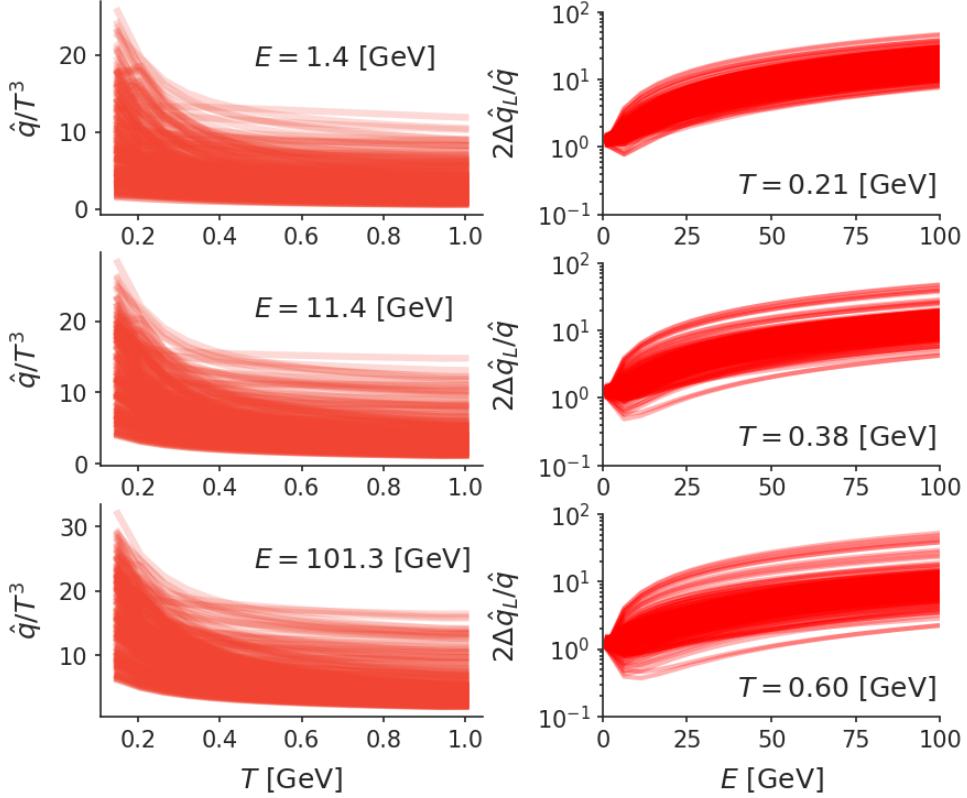


Figure 6.6 Left: the prior range of the transport parameter \hat{q} as function of temperature at different momentum. Right: the prior range of the longitudinal diffusion parameter \hat{q}_L , plotted as ratio $2\Delta\hat{q}_L/\hat{q}$.

previous benchmark calculation that the R_{AA} and v_2 predictions depends fairly weak on the choice of these parameter, therefore they are also given a logarithm prior. For the a and b parameters, one notice that asymptotically largeness or smallness of these numbers do not change the value of $\Delta\hat{q}$ notably. By applying the logarithmic prior and design, we can explore both the large and small limits of these numbers while still have enough design points to control the interpolation uncertainty in the physical interesting regions (a and b are of order one).

We sampled 250 design points and 50 validation points. Combining μ, K, p, q, a, b and γ , the prior region of the heavy quark transport parameters are plotted function of temperature and energy in figure 6.6. On the left, 250 design's \hat{q} as function of temperatures are shown (using charm mass for demonstration). Each subplot shows quark energy at 1.4 GeV, 11.4 GeV

and 101.3 GeV. The prior range of \hat{q} varies over an order of magnitude. On the right of the figure, we show the ratio $2\hat{q}_L/\hat{q}$ to indicated the degree of anisotropy of the transport parameters.

The computations of the model on both the design points and the validation points are performed on the NERSC super-computing system using over two million CPU hours. The prior observables are shown in figure 6.7 at LHC energy $\sqrt{s} = 5.02$ TeV and in figure 6.8 at RHIC energy $\sqrt{s} = 200$ GeV. In addition to LHC dataset used in the last calibration, we also include a dataset at RHIC energy measured by the STAR Collaboration [143, 144]. We choose two observables at RHIC, namely D meson R_{CP} and v_2 . The new one, R_{CP} , is defined as the N_{bin} normalized ratio between the D meson yield in a smaller centrality class C to a larger centrality class P ,

$$R_{CP} = \frac{dN_C/dp_T N_{\text{bin},P}}{dN_P/dp_T N_{\text{bin},C}}. \quad (6.6)$$

Using the nuclear data as a reference has the advantage of canceling certain theoretical uncertainties, such as the nuclear PDF (if its impact-parameter dependence is neglected) and possible modifications to the initial production mechanism in the nuclear environment. A problem we found at RHIC energy is that even varying wildly the parameters, the very low- p_T R_{CP} is not well covered by the calculation. This indicates the model will have to be improved in this region of p_T , possibly a more up-to-date dynamical hadronization model. Our temporary solution is to only include the STAR R_{CP} data above 5 GeV in the calibration.

Emulator validation The validation is performed by comparing the emulator trained on the 250 design points to the actual calculation on the 50 validation points. We visualize the validation in figure 6.9. In the top row, the emulated v_2 (left) and emulated R_{AA} (right) are compared with the model calculations, and the data from different experiments and centrality has been labeled by different colors. The emulated values strongly correlates with the true calculations around the the $y = x$ line. Most points hit off the line, meaning the emulator is not 100% accurate. To see if the uncertainty is accounted for, we scatter plot the emulator's prediction uncertainty (1σ , y axis) versus the absolute deviation between the prediction and the calculation (the x axis). The dashed line defines the shaded region where the true deviation is large than $\pm 3\sigma$. We found that over 99% of the prediction are within the 3σ region. Therefore, for most cases the emulator correctly estimates its uncertainty and therefore prevents over-fitting.

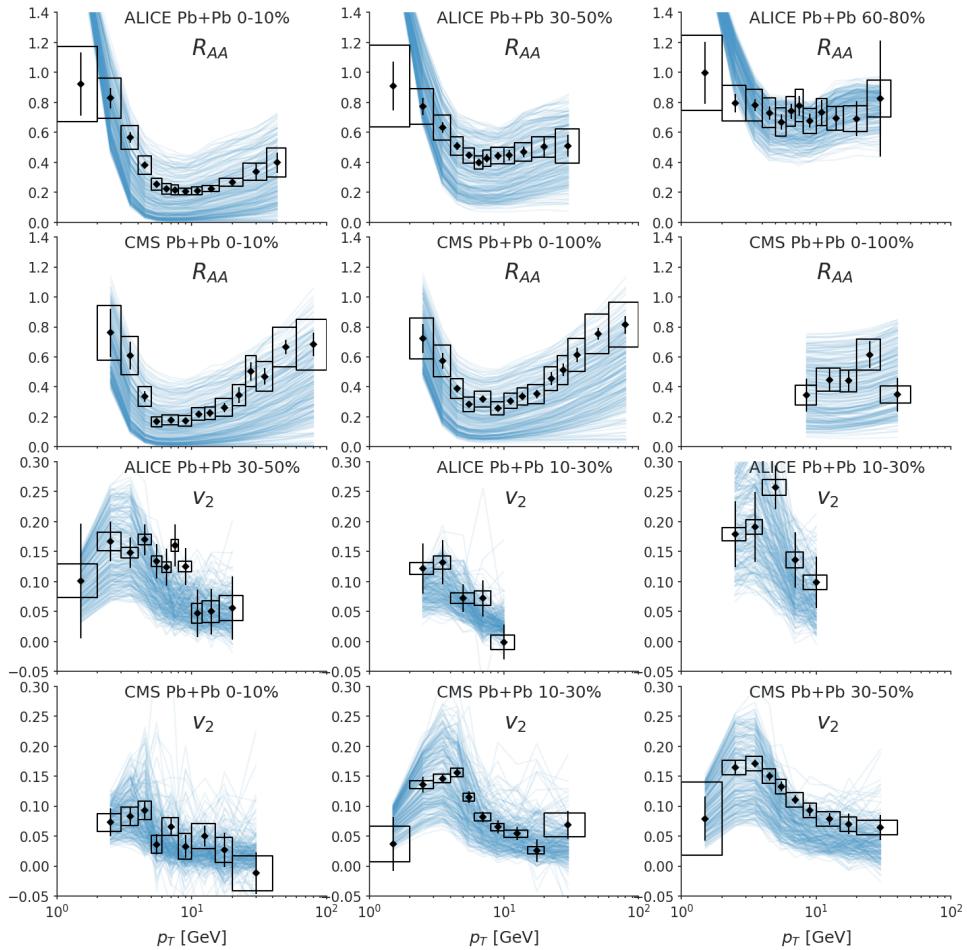


Figure 6.7 The prior distribution of the observables at the LHC energy.

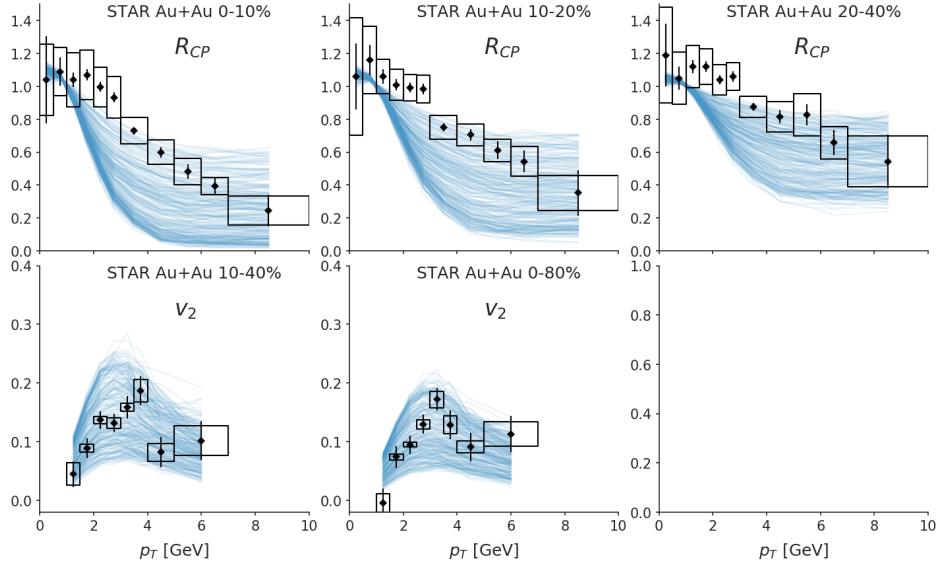


Figure 6.8 The prior distribution of the observables at the RHIC energy.

Co-variance matrix From chapter 5, the co-variance matrix has the structure

$$\Sigma = \Sigma_{\text{emulator}} + \Sigma_{\text{truncation}} + \Sigma_{\text{stat}} + \Sigma_{\text{sys}} + \Sigma_{\text{model, sys}} \quad (6.7)$$

The construction of these terms are straight forward, except for the systematic covariance Σ_{sys} of the experimental data. Usually, experiments publish the marginalized uncertainty on each observable point δy_{sys} (for example, R_{AA} of a certain centrality at a single p_T bin), and may specify the nature of the uncertainty as “correlated” or “uncorrelated”. The correlation among uncertainties is important as it directly affects the interpretation of the quality of fit. For instance: a fit with $+5\%$ deviations on each of the N data points will be penalized by a factor $e^{-N(0.05y)^2/\delta y^2}$, assuming uncorrelated uncertainty; while it will only be penalized by $e^{-(0.05y)^2/\delta y^2}$ if one assumes fully correlated uncertainty. This is because fully correlated uncertainty allows data to be systematically deviation from a trend.

However, we lack the information to construct the full covariance matrix from δy_{sys} . In this study, we simply parametrize the correlation as function of observables (labeled by $\alpha, \beta \in \{R_{AA}, v_2, R_{CP}\}$), centrality

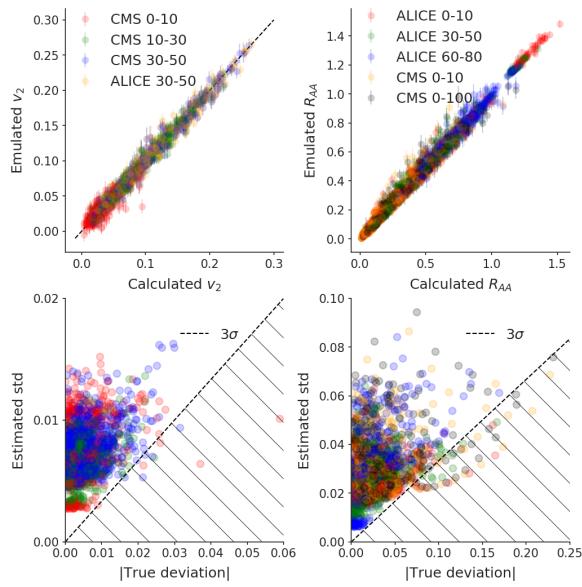


Figure 6.9 Validation of the emulators performance. The top two plots shows the correlation between the calculated quantities (x variable) versus the emulated quantities (y variable). The bottom two plots compares the GP's estimated standard deviation σ of the prediction to the true deviation from the actually calculation. The dashed regions indicates where the true deviations has a larger than 3σ difference from the emulator's prediction.

labeled by m, n and transverse momentum (labeled by i, j),

$$\Sigma_{\text{sys}} = \delta_{\alpha\beta} C_{mn} \exp \left\{ -\frac{1}{2L_{\text{corr}}^2} \left(\ln \frac{p_{T,i}}{p_{T,j}} \right)^2 \right\} \times \sigma_{\text{sys},i}^{\alpha m} \sigma_{\text{sys},j}^{\beta n}. \quad (6.8)$$

So, the covariance is zero if there are different observables or measurements from different experiments or different particle species. The centrality correlation C_{mn} is only applied to R_{AA} and R_{CP} as these quantities across different centrality shares the same baseline reference, so a fraction of their uncertainty must be correlated across-centrality. By default, $C_{m=n} = 1$ and $C_{m \neq n} = 0.3$. The correlation in the p_T dimension is assumed to be a Gaussian in the $\ln p_T$ space with correlation length L_{corr} . We use $\ln p_T$ based on the consideration that the original of these uncertainty should not be sensitive to the linear change of p_T as the there is no other scale present. The default correlation length is 1, meaning the uncertainty is effectively uncorrelated with measurements at a p_T 2.7 times larger or smaller. Finally, this correlation modulation is applied to the completely correlation case of the systematic uncertainty $\sigma_{\text{sys},i}^{\alpha m} \sigma_{\text{sys},j}^{\beta n}$.

This construction is entirely parametric, except for the direct experimental inputs $\sigma_{\text{sys},i}^{\alpha m}$. We hope that future measurements will provide more information on the co-variance structure of the published systematic uncertainties. In the actually calibration, we will also change a few default parameters to see if the extracted physical parameters are sensitive to the detailed construction of Σ_{sys} .

Posterior observables The global level of agreement between the calibrated model and the data is shown in figure 6.10 at the LHC energy, and figure 6.11 at the RHIC energy. The black dashed lines show the median prediction, while the blue bands stands for 90% credible region. We remind the reader that because of the model predicts anti-correlation between R_{AA} and v_2 , the lower and upper bounds of the uncertainty bands are also anti-correlated. For example, a line that is close to the higher bounds in R_{AA} is likely to be lose to the lower bounds in v_2 .

Both the D -meson and the B -meson R_{AA} at the LHC energy are well described by the calibrated model, while v_2 is systematically below the data. Large separation between the event-engineered v_2 is observed, At the RHIC energy, v_2 has a better agreement. The magnitude of R_{CP} at $p_T > 5$ GeV¹ and its centrality dependences is correctly reflected, though the shape is too flat compared to the data.

¹Remember that the model is calibrated on the three data points above $p_T = 5$ GeV

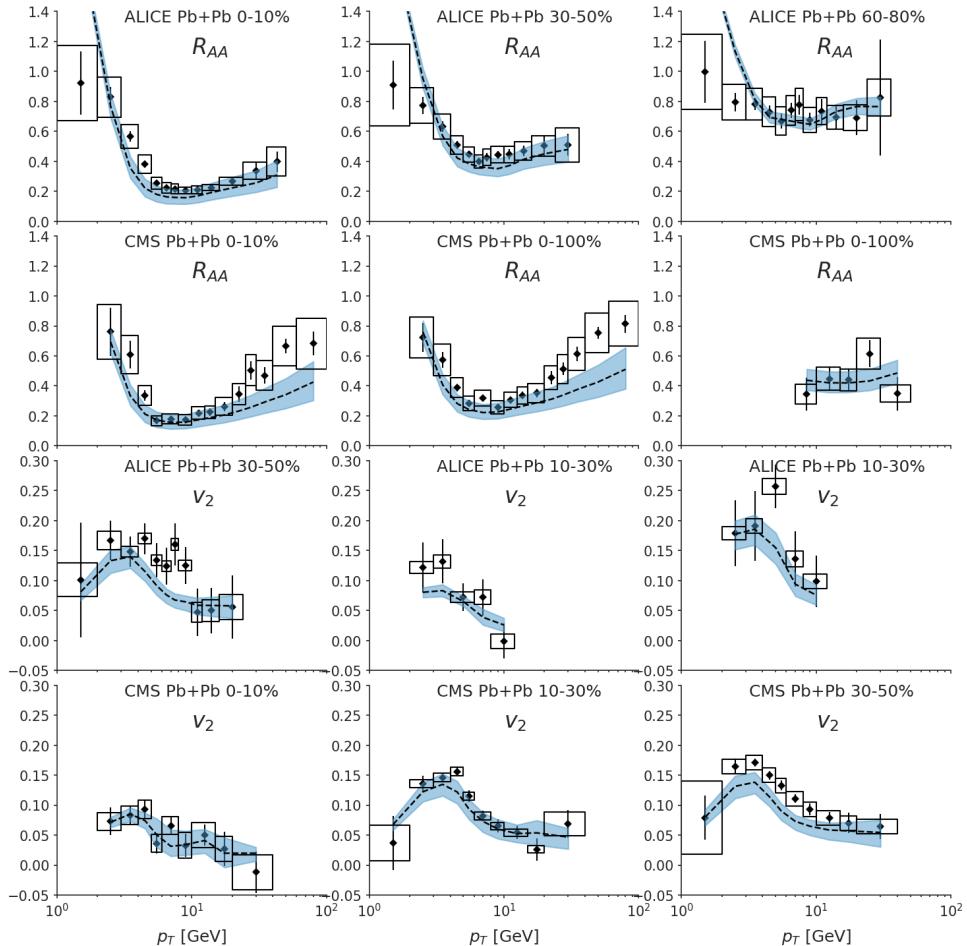


Figure 6.10 The 90% credible region (blue bands) of the posterior distribution of the observables at the LHC energy. Black dashed lines are the median prediction.

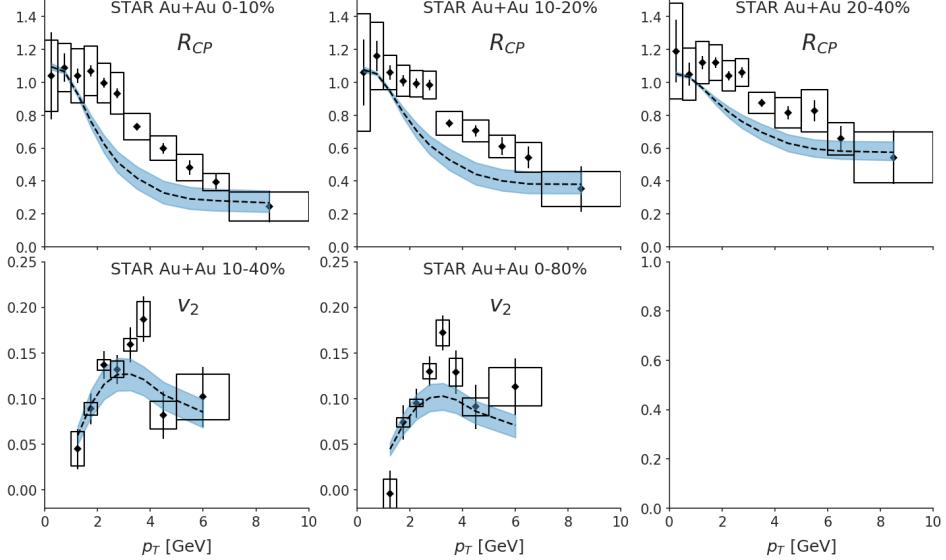


Figure 6.11 The 90% credible region (blue bands) of the posterior distribution of the observables at the RHIC energy. Black dashed lines are the median prediction.

Posterior distribution of parameters Figure 6.12 shows the single parameter posterior (diagonal plots) and two-parameter-joint posterior distributions (off-diagonal plots) of the 10 model parameters, plus the model systematic uncertainty parameter (σ_m). The $\ln \mu$ parameter has an evident peak around 1.3, which corresponds to $\mu \approx 3.5$. The resulting posterior of α_s is plotted in figure 6.13, the median value of α_s at $Q = \mu\pi T$ varies from 0.3 to 0.22 for the relevant temperature range $0.15 < T < 0.5$ GeV, corresponding to $g \sim 2$. Note that this α_s does not stand for the strength of all the probe-medium interaction, recalling that there is a significant parametric diffusion contribution to the elastic energy loss. For radiative process, though the $1 \rightarrow 2$ splitting vertex explicitly uses this α_s , the strength of the LPM effect is again controlled by the elastic broadening. Compared to the previous extraction, the preferred in-medium coupling strength is smaller and is closer to the phenomenological values used by other studies [145]. However, the coupling is still large compared to the weakly coupled assumption $g \ll 1$.

The energy loss starting is preferred to be after about half of the hydrodynamic starting time. The switching scale parameter do not have a strong preference as long as it is not too large, which is consistent with our model construction that physical processes should be weakly depends on

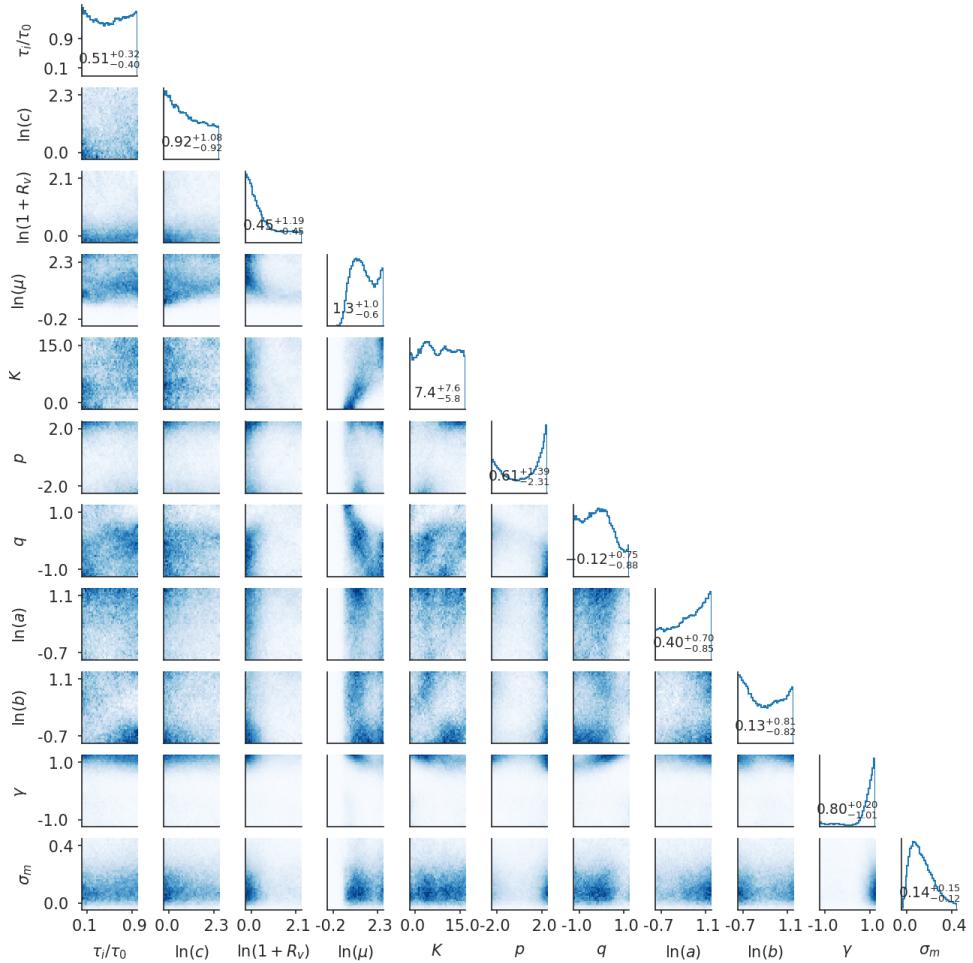


Figure 6.12 The single-parameter posterior distributions (diagonal plots) and two-parameter joint posterior distributions (off-diagonal plots).

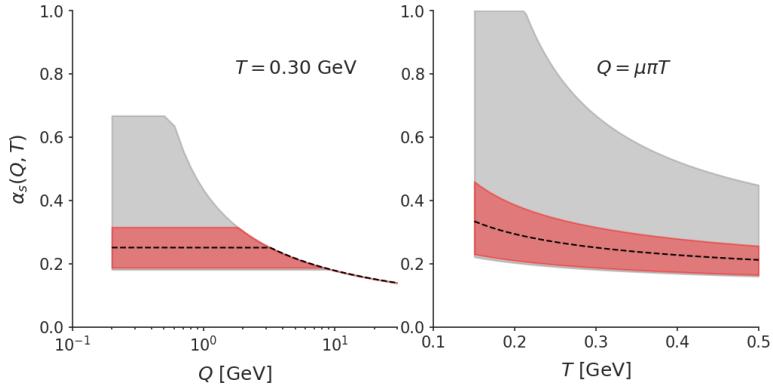


Figure 6.13 Left plot: the scale dependence of the running coupling constant at $T = 0.3$ GeV. Right plot: the temperature dependence of running coupling evaluated at the cut-off scale $Q = \mu\pi T$. The red bands are generated using 90% credible region of the μ parameter; the gray bands are the prior distributions; and the black dashed lines are median predictions.

this switching scale between diffusion and scattering modeling. The matching parameter R_v is not very well constrained, but tends to prefer a smaller value.

We plotted the 90% credible range (red bands) of the posterior transport parameters \hat{q}, \hat{q}_L on top of their prior range (gray band) in figure 6.14. The transport parameters is nicely constrained and is comparable to the earlier extraction by the JET Collaboration ². We also present a first extraction of the longitudinal transport parameter \hat{q}_L . The longitudinal transport is quite anisotropic when compared to \hat{q} . First, its perturbative contribution already introduces

For the heavy quark spatial diffusion constant, since it is related to \hat{q} in the zero momentum limit. Such an extraction is essentially an extrapolation of our parametrization, and can be sensitive to the detailed choice of the ansatz. Nevertheless, the extraction is (red band for 90% credible region) is compared to varies lattice calculations [146–148] in figure 6.15. Our extraction for both charm and bottom quark spatial diffusion constants is similar, and is consistent with lattice calculations in the static / infinitely heavy limit of the heavy quark. While the lattice calculation of dynamical charm quark gives a much lower value of D_s . One may expect that our phenomenological extraction should give a similar separation between bottom

²Note that the JET Collaboration extracts the light quark \hat{q} . However, at $p_T = 10$ GeV, the mass effect of the charm is small and these two numbers should be comparable.

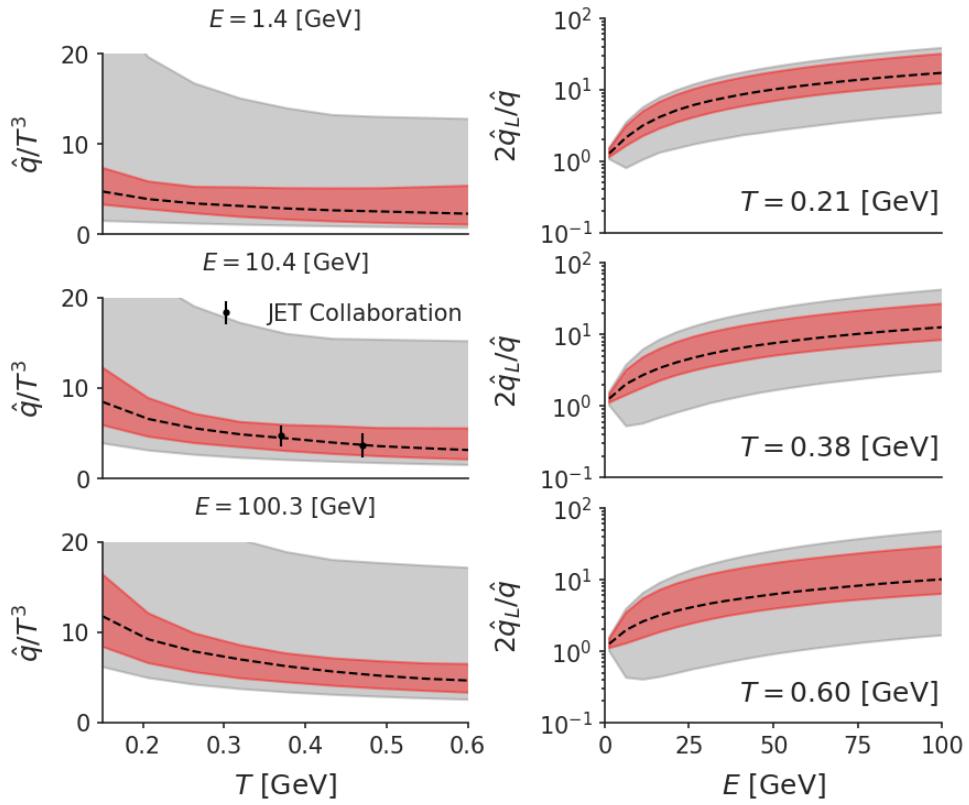


Figure 6.14 The 90% credible region of the charm quark transport coefficients (left plot) and of the longitudinal transport parameter (right plot) are shown in red. The prior range are shown in gray. The results are also compared to the previous JET Collaboration extraction of the light quark transport parameters at $p = 10$ GeV (black symbols).

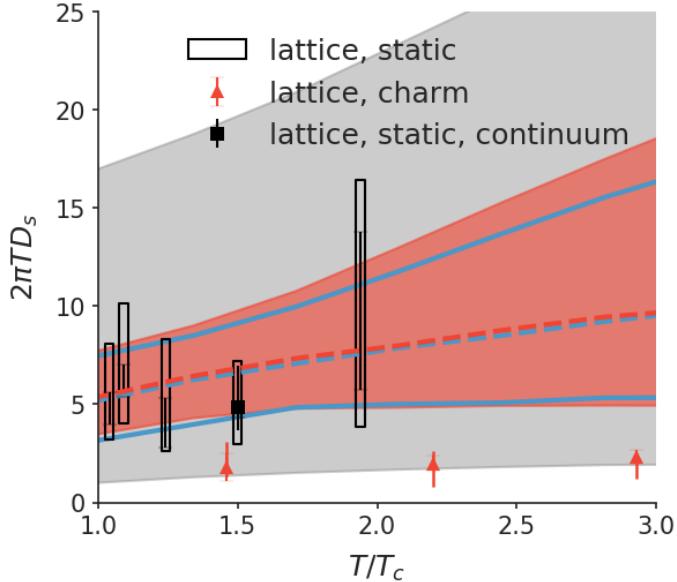


Figure 6.15 The 90% credible region of the spatial diffusion constant defined in the zero momentum limit. Prior range is indicated by the gray band. The posterior of charm and bottom flavor are shown as red band and blue boundary respectively. It is compared to lattice QCD evaluation in references [146] (black boxes), [148] (the black dot) and [147] (red triangles).

and charm flavor, as the bottom is more than three times heavier. However, we found that the mass dependence in the elastic part of our model is relatively weak. First, the mass only affects the phase-space integration of t -channel exchange perturbative scattering. Second, the diffusion parameter of the weakly coupled theory, we are using explicitly heavy-quark limit that it does not depend on mass. Finally, mass only enters the parametric diffusion part through a combination E/T , which is approximately M/T at low momentum, since both charm and bottom mass are already much higher than the typical temperature, the parametric part also introduces a weak flavor dependence. In the future, one may seek for more physically motivated flavor dependence parametrization of the transport parameters.

7

Conclusion

As a summary this dissertation, I focus on understanding the transport property of the heavy flavor in the strongly coupled quark-gluon plasma applying model-to-data comparison methodology, aiming for model improvements and uncertainty quantification.

A prerequisite for the study in an “accurate” modeling of the physical ingredients to be tested. It is not so trivial to model the heavy quark transport that is coupled to an event-by-event fluctuating and evolving medium. On the one hand, this is because the finite medium-induced radiation formation time at high energy is much greater than the mean-free-path in semi-classical transport equations, and can be comparable to the medium evolution time scales. On the other hand, there are two compelling pictures regarding the heavy-quark-to-medium coupling: weakly coupled picture modeled by scatterings, and strongly coupled picture whose dynamics is often modeled by diffusion equations. We developed a transport model for hard parton propagation in near equilibrium plasma. An improved treatment of LPM is implemented and it is shown to reduces to theoretical calculations in idealized infinite static medium limit, and captures qualitative features in a finite and evolving medium. The model also treats the large and small momentum transfer processes with different strategies of few-body scattering and diffusion (plus diffusion-induced radiation) method, which grants flexible parametrization of diffusion-like deviations from leading order weakly coupled approach.

The transport in hot QGP stage fits into a more general “transport” picture including the initial production and high-virtuality evolution, hadronization near the transition temperature and decay and hadronic dynamics. We identity a matching problem between the high-virtuality evolution and

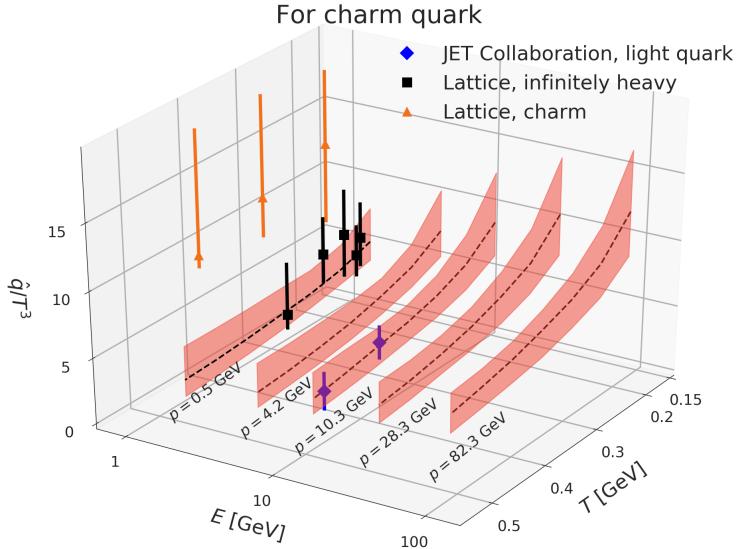


Figure 7.1 This figure shows the main result of this dissertation. The 90% credible transport coefficient \hat{q}/T^3 extracted for the charm flavor is displayed on the two dimensional landscape of energy and temperature. The JET Collaboraton extraction of light quark transport coefficients at $p = 10 \text{ GeV}$ [145] (blue diamonds) and two lattice calculations of the momentum diffusion coefficient κ ($\hat{q} = 2\kappa$) [146, 147] are plotted for comparison.

medium-induced evolution. Currently, a unified formulation that smoothly connecting the virtuality shower and the in-medium shower is still missing, and we use a separation of phase-space to terminate vacuum showers at a scale (Q^2) where it is likely to receive similar amount of medium modifications to the transverse momentum ($\Delta k_\perp^2 \sim Q^2$). The exact location of the separation scale is then treated as an uncertainty of the model.

Finally, we apply the Bayesian analysis to infer the model parameter distribution by comparing to heavy flavor measurements at both RHIC and the LHC. The model parameters includes uncertainties such as in-medium coupling strength, energy loss starting time, match scale between vacuum and medium-induced shower, diffusion versus scattering model, as well as parametrized deviations from weakly coupled calculations.

We highlight the progress of this work in the conclusion figure 7.1. It visualizes 90% credible region of the energy and momentum dependence of the heavy quark momentum diffusion transport parameter \hat{q} scaled by T^3 . We found \hat{q}/T^3 gradually increases with $\ln E$ and displays an enhance-

ment near the critical temperature. Studying heavy flavor helps to connect the knowledge of in-medium transport properties at very high momentum (light limit) and very low momentum (static sources limit). At relatively high momentum $p \sim 10$ GeV, it is consistent to the light quark transport parameter extracted by the JET Collaboration (blue). At low momentum $p \sim 0.5$ GeV, it is consistent with lattice calculations in the heavy quark limit (black). Future study with improved flavor dependence may be needed to understand the impact of using the “heavy” limit in dynamical model. In the current present calibration, the effective in-medium strong coupling constant is about 0.3, and only contribute a small fraction of the extracted \hat{q} parameter. The rest comes from the parametric contribution whose origin can be either perturbative or non-perturbative; either way, it suggests the necessity to model beyond leading order physics.

In conclusion, a transport modeling with perturbative based parton evolution with a parametric probe-medium interaction term is able to describe a wide range of open heavy flavor data to about 30% level of accuracy. The heavy quark transport properties as function of energy and temperature is consistent with early phenomenological studies and lattice calculation. The present level model accuracy is still not enough to make the best use of future high-precision hard probe measurements in heavy-ion collisions. We therefore summarize a few points of improvements in the end which may help to reduce or estimate the theoretical and modeling uncertainties.

- An interpolation formula between vacuum and medium-induced radiation. A calculation that connects virtuality evolution with in-medium time evolution will help to eliminate the matching scale uncertainty. Though for the present observable and p_T range its effect is not strong, its treatment may impact more delicate jet observables.
- Correlation among multiple emissions in the presence of medium. We have been neglecting the correlation among subsequent emissions in the “modified transport model”. In the infinite medium limit, this is because the probability of overlapping emissions scales as $\tau_{1,f}R(\omega_2) \sim \tau_{1,f}\alpha_s/\tau_{2,f}$ which is suppressed by α_s . But this higher order effect can be important since the phenomenological α_s is not small. There has been ongoing studies on this subject.
- Off equilibrium correction to the linearized transport equation. One essential assumption in linearized transport model is that medium partons follow the local thermal distributions, even though the hydrodynamics is propagated with viscous corrections. In fact, the viscous cor-

rection and the momentum space anisotropy can be very large at early times of the hydrodynamic evolution. One need to understand how these off-equilibrium effects changes the interpretation of the transport parameter one extracted assuming full thermal equilibrium of partons.

- Dynamical hadronization model and improved treatment of energy loss in the hadronic stage. Our current hadronization model has the problem of pinching long distance physics into a sudden process. At low- p_T , the sudden recombination model breaks the detailed balance of the transport model and treating recombination model in a dynamical way would be more suitable. At high- p_T , the problem is more severe, as the hadronization time scale is dilatation by the large boost. Moreover, the hadronic system near T_c is still very dense, and it is inconsistent to apply the vacuum fragmentation function at the moment $T \sim T_c$. One possible solution for those high- p_T heavy quarks (the recombination process is negligible) is to continue their partonic transport into the hadronic phase, and finally apply the vacuum fragmentation function when the system is dilute enough. Meanwhile, one can also study the energy loss in the dense hadronic system to extend the extracted transport parameter to the region below T_c .
- A calibration with simultaneous tuning bulk and hard sector. The bulk medium calibration is performed by a separate analysis. With future high precision hard probe measurements, a simultaneous calibration of both soft and hard sector would be interesting. For example, we found that the number of binary collision as function of centrality is quite sensitive to the proton shape modeling in the Monte-Carlo Glauber model. The sensitivity of hard production to the number of binary collision may help the soft sector to improve the proton shape modeling. In turn, a better calibrated medium help to reduce the uncertainty in the hard parton energy loss.

dissertation

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