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Medium effects in small systems

The bigger picture of heavy ion collisions

Le Roux, Chiara

2025

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Citation for published version (APA):

Le Roux, C. (2025). *Medium effects in small systems: The bigger picture of heavy ion collisions*. Lund University.

Total number of authors:

1

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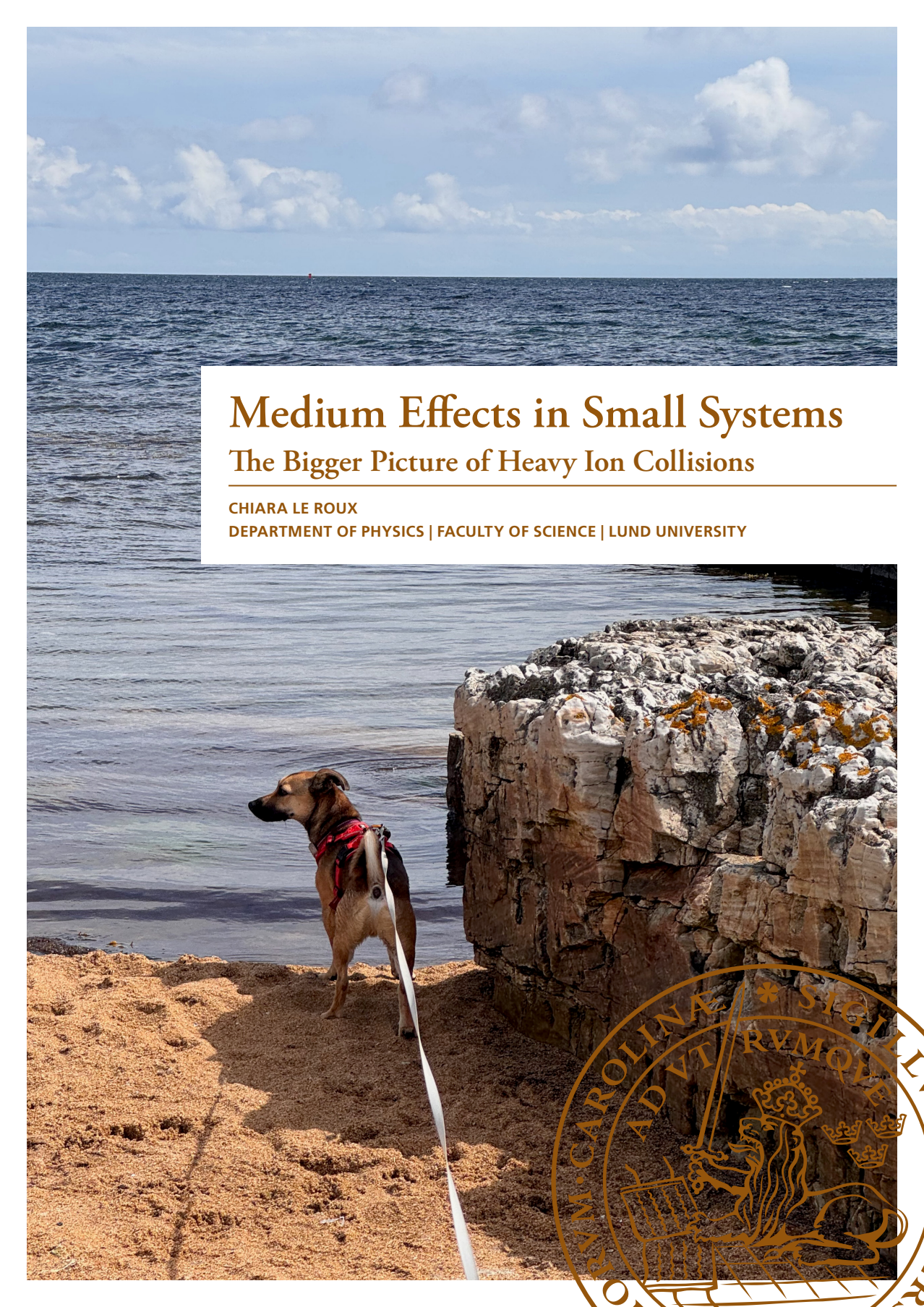
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Medium Effects in Small Systems

The Bigger Picture of Heavy Ion Collisions

CHIARA LE ROUX

DEPARTMENT OF PHYSICS | FACULTY OF SCIENCE | LUND UNIVERSITY



Medium Effects in Small Systems
The Bigger Picture of Heavy Ion Collisions

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The Bigger Picture of Heavy Ion Collisions

by Chiara Le Roux



LUND
UNIVERSITY

Thesis for the degree of Doctor of Philosophy

Thesis advisor: Korinna Zapp

Faculty opponent: Konrad Tywoniuk

To be presented, with the permission of the Faculty of Science of Lund University, for public criticism in Rydbergsalen at the Department of Physics on Friday the 5th of December 2025 at 13:15.

Organization LUND UNIVERSITY Department of Physics Professorsgatan 1 SE-223 63 LUND Sweden		Document name DOCTORAL DISSERTATION
Author(s) Chiara Le Roux		Date of disputation 2025-12-05
		Sponsoring organization
Title and subtitle Medium Effects in Small Systems: The Bigger Picture of Heavy Ion Collisions		
Abstract The main focus of this thesis is on the puzzle of small systems, which arose when several signatures of the medium of quarks and gluons formed in heavy ion collisions were also observed in collisions of small systems, except for jet energy loss. To understand why that could be happening, papers I, III and IV focus on quantifying the sensitivity of different observables to medium interactions, whereas paper II explores another origin of anisotropies in small systems. Paper I quantifies the dependence of R_{AA} and v_2 on jet-medium interactions. It focuses on these two observables as they are commonly used to search for jet quenching and collective behavior respectively. We found that, while both of these observables scale with the average momentum transfer at each scattering, they can be affected in different ways depending on the stage of the parton shower evolution in which the scattering takes place. Paper II builds a new Glauber model for pA collisions. It does so by implementing new nucleon-nucleon cross-sections calculated within the KMR/SHRiMPS model, which presents a well motivated calculation of soft QCD observables. It was shown that, this new cross-section model, which contains a non-trivial impact parameter dependence, can account for fluctuations that other commonly used Glauber models often neglect. Moreover, it was shown that such fluctuations have a great impact in the spacial anisotropy of the initial conditions. Paper III explores the formation time of jets, τ_f, as a probe for color coherence. In this paper, it was demonstrated that τ_f is sensitive to decoherence, which may be caused, for example, by interactions with a medium even when they are so soft that energy-momentum transfer is negligible. Therefore, it can be used as a probe for medium effects in systems where no jet quenching is observed. Paper IV also focuses on coherence effects in small systems. In this case, we focus on systems where energy loss can be seen, and we investigate how it might be modified by color coherence.		
Key words Heavy ions, jet quenching, small systems, color coherence.		
Classification system and/or index terms (if any)		
Supplementary bibliographical information		Language English
ISSN and key title		ISBN 978-91-8104-632-8 (print) 978-91-8104-633-5 (pdf)
Recipient's notes	Number of pages 131	Price
	Security classification	

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Medium Effects in Small Systems

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A doctoral thesis at a university in Sweden takes either the form of a single, cohesive research study (monograph) or a summary of research papers (compilation thesis), which the doctoral student has written alone or together with one or several other author(s).

In the latter case the thesis consists of two parts. An introductory text puts the research work into context and summarizes the main points of the papers. Then, the research publications themselves are reproduced, together with a description of the individual contributions of the authors. The research papers may either have been already published or are manuscripts at various stages (in press, submitted, or in draft).

Cover illustration front: My dog Zuko photographed by me, 2025.

Cover illustration Paper I: Photo taken by me at *Kiyomizu-dera* in Kyoto during my trip to Japan for the Hard Probes conference, 2024.

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Cover illustration Paper III: Photo I took at *Mont-Saint-Michel* when I went to Normandy for the QCD Masterclass Summer school, 2023.

Cover illustration Paper IV: Photo of my dear friends taken by me in Stockholm in our trip to attend Partikeldagarna, 2024.

Cover illustration back: Photo of the *Aurora Borealis* taken by me during a trip to Kiruna, 2025.

Funding information: This work is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 803183, collectiveQCD).

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Faculty of Science, Department of Physics

ISBN: 978-91-8104-632-8 (print)

ISBN: 978-91-8104-633-5 (pdf)

Printed in Sweden by Media-Tryck, Lund University, Lund 2025



*To all the little girls
who will be great
scientists one day.*

“But my ideas in my head aren’t the only ones important to me. My society is also an idea. I was made by it. An idea of freedom, of change, of human solidarity, an important idea. And though I was very stupid I saw at last that by pursuing the one, the physics, I am betraying the other.”

— Ursula Le Guin, *The Dispossessed*

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Acknowledgements

After this long and difficult process, I realize that it takes a village to finish a thesis. I would not have enough pages to cite all the names that contributed to me being able to complete this work. Instead, I choose to mention the names of those without whom there probably would have been no thesis or, at least, there would have been one with only a fraction of the quality.

First and foremost, I thank my mother, Rossana, without whom I could not even imagine this to be possible. My father, Galo, and my two brothers, Nicolas and Felipe, were also at the very core of the process that turned this into reality. Thank you as well to my grandmother, Gilda, my grandfather Carlos, my aunt Susi and my four-legged sibling, Caju. Obrigada.

My partner Lucas was not only my greatest example of perseverance and strength, but also my biggest supporter. I have no words to describe how thankful I am to you. Thank you also for embarking on this crazy journey of adopting our beloved Zuko in the middle of all of this. There is nothing like an adorable puppy to make us get our heads out of thesis writing and go for an energizing walk.

I would like to thank the immense support of my supervisor Korinna Zapp. Thank you for being so understanding and supportive throughout these years. I must say I learned an incredible amount of physics with you, but also so much more. Thank you for being such an inspiring example. Thank you also for helping me make connections with our collaborators for the papers in this thesis: Guilherme, Liliana and Isobel also have my endless gratitude. Thank you for all the fun discussions, cool projects and, especially, for being so understanding of my deadlines and helping this thesis come to life.

I must also thank Christian Bierlich for such a detailed reading of my thesis and the many constructive comments that made this text so much better. Thank you also to all the seniors in the division for all the support and advice. A special thank you to Leif Lönnblad and Christian Bierlich for the times I knocked on your doors to chat about physics. The same goes to Alice Ohlson, who so patiently answered so many of my questions. My past mentors also deserve a special mention for preparing me so well for this arduous task of completing a PhD: Fernando Navarra, Marco Bregant and Hugo Natal da Luz, muito obrigada.

I cannot emphasize enough how thankful I am to all my junior colleagues with whom I shared many lunches, fikas, board game nights, movie nights and many other fun events. I will not dare mention all of your names, but without your encouragement, and all our venting and laughing sessions, this thesis would not have been possible. A special thank you goes to two of my office mates and friends, Belikse and Robin, who lent me their ears (and, at times, their shoulders) so many times throughout these years. Thank you also to Andy for so much encouragement and support, both in PhD work and in dog caring. Finally, if you have been in this division at any time in the past two years, you know that the person that has been there for me the most, no matter what and with no questions asked is Anca. I am so extremely grateful for your support and friendship, it has literally changed my life. Thank you so much.

I also could not have made it without the help of the administrative and IT personnel at this division. A special thank you to Eva Jurlander, Karin Lennebo, Minna Ramkull, and Florido Paganelli for all the assistance and patience.

I must also thank the friends that were there for me way before I could ever imagine doing a PhD. Thank you Tathi, Luana, Bia and Deby, who have been my support pillars throughout many of my past achievements and continued to bear with me in this process of getting a PhD. Thank you also to all my other friends in Brazil who were part of this journey. A special thank you goes also to Isabella for being not only an amazing and supportive friend but also my conference and Summer school buddy for the past four years. I must also acknowledge all the colleagues and friends whom I have met throughout the workshops, conferences and Summer schools, you made this adventure so much more delightful. Special shout out to the big group of Brazilians that I was always sure to encounter and feel immediately at home at any event that I attended. Thank you for all the shared experiences and for being an outlet for all the feelings that only those who know what it is to be an immigrant can understand. Along these lines, I would also like to thank the group of Brazilians I immediately found upon moving to Sweden, in special Tamires and Henrique, thank you for welcoming me here and for letting my dog play with your dogs.

Lastly, I would like to thank all the professionals and volunteers working on so many projects that are dear to me and that I myself keep postponing in order to pursue yet another degree. Thank you in special to Amigos Mios, Rovers Rescue and all other animal rescues that are out there saving lives.

List of publications

This thesis is based on the following publications:

- I How many interactions does it take to modify a jet?**
Chiara Le Roux, José Guilherme Milhano, Korinna Zapp
Eur. Phys. J. C 85, 1065 (2025)
e-print: arXiv:2412.14983 [hep-ph]

- II How cross section fluctuations affect multiplicity and geometry in pA collisions**
Chiara Le Roux
Submitted to Eur. Phys. J. C
e-print: arXiv:2507.21843 [hep-ph]

- III Jet quenching without energy loss**
Liliana Apolinário, Chiara Le Roux, Korinna Zapp
Submitted to Phys. Lett. B
e-print: arXiv:2510.11914 [hep-ph]

- IV Colour coherence in small collision systems**
Isobel Kolbé, Chiara Le Roux, Korinna Zapp
To be submitted
e-print: arXiv:2510.17570 [hep-ph]

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Resumo em português

Ao longo da História, os seres humanos tentaram compreender e descrever o mundo ao seu redor e do que ele é feito. Muitas destas tentativas consistiram em encontrar ingredientes fundamentais que pudessem ser combinados de diferentes maneiras para formar toda a matéria que observamos — desde a terra sobre a qual pisamos até as estrelas que vemos no céu. Séculos depois, tais esforços culminaram em uma das teorias mais bem-sucedidas da Física: o Modelo Padrão da Física de Partículas.

De acordo com esse modelo, existem 12 partículas que são as unidades elementares da matéria. Essas partículas interagem e combinam entre si por meio de três interações possíveis (além da gravidade): as interações eletromagnética, fraca e forte. Cada um desses três tipos de interações possui comportamentos e características diferentes e, portanto, dá origem a diferentes tipos de fenômenos. Assim, diferentes estratégias devem ser utilizadas no estudo das diferentes interações. O foco desta tese está em uma dessas estratégias — mais precisamente, em uma que nos permite estudar fenômenos específicos das interações fortes. Em outras palavras, o foco é a fenomenologia das colisões de íons pesados relativísticas.

Para entender o que isso significa, vamos analisar mais de perto a estrutura da matéria. Se perguntarmos a um químico do que a matéria é feita, ele dirá que é composta por átomos. No entanto, estes não são estruturas fundamentais: eles são formados por um núcleo e uma “nuvem” de elétrons ao seu redor. O núcleo é responsável pela maior parte da massa do átomo, enquanto a nuvem de elétrons ocupa um volume muito maior. Como isso é possível? Isto ocorre por causa da composição elementar do núcleo, que é formado por partículas que interagem por meio da força forte. Esta força permite que elas fiquem densamente compactadas dentro dos núcleos atômicos. Portanto, se o objetivo é estudar as interações fortes, faz sentido focar nos núcleos dos átomos. Portanto, assim como uma criança desmonta um brinquedo para entender como ele funciona, um físico quebra os núcleos dos átomos para compreender seu funcionamento interno.

Uma das estratégias para estudar a interação forte consiste, então, em remover os elétrons de átomos pesados (criando assim íons pesados), acelerá-los a velocidades próximas à da luz (velocidades relativísticas) e colidi-los entre si. Essas são as colisões de íons pesados relativísticas. Quando isso é feito, o resultado é que os núcleos quebram em seus ingredientes fundamentais: partículas elementares chamadas quarks e glúons. Devido às condições extremas em que isso ocorre, as densidades e temperaturas às quais a matéria é submetida são tão incrivelmente altas que esses quarks e glúons formam um novo estado da matéria. Esse estado só poderia existir naturalmente logo após o Big Bang, quando o Universo era quente e denso o suficiente para que ele existisse. Assim, ao colidir íons pesados a velocidades relativísticas, podemos estudar as propriedades desse novo estado da matéria.

Há décadas, estes experimentos vêm sendo realizados em diferentes laboratórios ao redor do mundo (especialmente no LHC, localizado no CERN, e no RHIC, que fica no BNL), e esse novo estado da matéria, chamado de “Plasma de Quarks e Glúons” (QGP, na sigla em inglês), já foi detectado e teve suas características estudadas. No entanto, quando certas assinaturas do QGP também foram observadas em colisões de íons leves — que, em princípio, não deveriam ser densos o suficiente para recriar as condições do Universo primordial

—, alguns desses resultados passaram a ser questionados. Esse é o chamado “*puzzle of small systems*”, ou “dilema dos sistemas pequenos” em tradução livre.

Esta tese foca justamente neste dilema. Isto é feito principalmente por meio de simulações de Monte Carlo. As simulações permitem testar hipóteses teóricas de maneira que possam ser comparadas diretamente com observações experimentais. Assim, essas foram as ferramentas utilizadas nesta tese para compreender a fenomenologia dos sistemas de colisão pequenos e grandes utilizando uma base teórica unificada dentre todos os sistemas estudados.

Popular summary in English

Throughout History, humans have tried to understand and describe the world around them and what it is made of. Several of these attempts have consisted in finding common building blocks which can be combined in different ways to form all the matter we see: from the earth we stand on to the stars we see in the sky. Centuries later, such attempts have culminated in one of the most successful theories in Physics: the Standard Model of Particle Physics. According to this model, all matter is composed of 12 particles, which are the elementary units of matter. These particles combine by interacting with each other via three possible forces (apart from gravity): the electromagnetic, weak and strong forces. Each one of these three types of interactions have different behaviors and characteristics and, therefore, they give rise to different kinds of phenomena. Thus, in order to study them, different strategies should be applied. The focus of this thesis is on one of these strategies, more precisely, one that allows us to study specific phenomena to the strong interactions. In other words, the focus is the phenomenology of relativistic heavy ion collisions.

To understand what that means, let us zoom in on the structure of matter. If asking a chemist what matter is made of, they will say that matter is made of atoms. However, these are not fundamental structures. They are actually made of a nucleus and a “cloud” of electrons around it. The nucleus is responsible for the majority of the mass of the atom, whereas the electron cloud spreads out over a much larger volume. How can that be? Well, this is because of the elementary composition of the nucleus, which is made of particles that interact via the strong force mentioned above. This allows them to be compactly packed inside the atoms’ nuclei. Therefore, if one aims at studying the strong interactions, then one should look at the nuclei of atoms. More precisely, just as a child might disassemble a toy to learn how it works, a physicist will break up the nuclei of atoms to understand its inner workings.

Therefore, one strategy to study the strong interaction, is to remove the electrons from heavy atoms (thus creating heavy ions), accelerate them to almost the speed of light (relativistic speeds) and collide them with each other. These are the relativistic heavy ion collisions. When this is done, the result is that the nuclei will get broken into their most fundamental building blocks: elementary particles called quarks and gluons. Given the extreme conditions in which this happens, the densities and temperatures that the matter is subjected to are so incredibly large that these quarks and gluons will form a new state of matter. This state of matter could only exist naturally right after the Big Bang, when the Universe was hot and dense enough for that. Therefore, by colliding heavy ions at relativistic speeds, scientists can study the properties of a new state of matter.

For decades these experiments have been taking place in different facilities around the world (notably in the LHC at CERN and the RHIC at BNL) and this new state of matter, named the “Quark and Gluon Plasma” (QGP), has been detected, and its characteristics have been thoroughly studied. Nevertheless, when certain signatures of the QGP were also observed in the collision of light ions, which, in principle, should not be dense enough to recreate the conditions of the early Universe, some of these findings have been questioned. This is what is known as the puzzle of small systems. This thesis sheds a light on precisely

this puzzle by using Monte Carlo simulations of such collisions. The simulations allow us to put theoretical assumptions to test in ways that can be directly compared to experimental observations. Therefore, those were the tools used in this thesis to understand the phenomenology of small and large collision systems in a unified coherent framework.

Introduction

There was process: process was all. You could go in a promising direction or you could go wrong, but you did not set out with the expectation of ever stopping anywhere.

— Ursula Le Guin, *The Dispossessed*

In this thesis I will present the main findings from my studies of the past four years. During these years, I took a deep dive into the phenomenology of relativistic heavy ion collisions and, before going into the actual content, I take this opportunity to briefly reflect on how my journey in physics lead me to this thesis.

The first physics course that fascinated me and lead me to make a pivotal change in my career choice was electromagnetism. I believe that was one of the first opportunities I had contact with the concept of fields. I found it extraordinary that common phenomena from our day-to-day can be explained by the presence of electromagnetic fields. How those entities silently surround us and how their presence manifests itself in mundane situations such as, for example, the loud interruptions of the many thunders of a cozy Summer afternoon storm in my hometown in Brazil. Although this sounds trivial to me today, I remember how non-intuitive it seemed when I first understood that physical objects can be described by fields, which simply meant that they have some value at any point in space-time and that this value can be a number, but it can also be a vector, or even a more complex mathematical structure. The point is that what called my attention in the electromagnetism course were these concepts that are directly connected to tools I would need later on when studying particle physics.

However, the most game changing concept introduced to me in that occasion was that of symmetry. Of course, I knew what symmetry was before going into higher education, but I had not imagined that a simple apparently aesthetical concept could have such impactful consequences in physics. Symmetry is a fundamental concept in particle physics and the basis for the Standard Model, which is known as one of the most successful models in physics and, perhaps, the closest we have to a “theory of everything”. It is one of the symmetries in the Standard Model, the so-called color $SU(3)$ (more on that later), which is responsible for all the phenomenology that is in the core of this thesis. The collision of relativistic heavy ions is nothing but a way to study the consequences of this symmetry on

the theory of elementary particles.

With that, we shall get into the contents of the thesis starting with a brief discussion of the SM in section 1. Then, section 2 gives an overview of the phenomenology of heavy ion collisions. This is followed by a discussion of the tools used in the works within this thesis in section 3. Finally, the papers resulting from this work are reproduced at the end.

I The Standard Model of Particle Physics

*Rien ne serre le cœur comme la symétrie. C'est que la symétrie c'est l'ennui, et l'ennui est le fond même du deuil. (...) On peut rêver quelque chose de plus terrible qu'un enfer où l'on souffre, c'est un enfer où l'on s'ennuierait.**

— Victor Hugo, *Les Misérables*

The Standard Model (SM) of particles physics offers an answer to the centuries old question: “what are things made of?”. It presents the fundamental particles that form the building blocks of all the visible matter in the Universe and organizes them into the simple and compact table shown in Fig. 1. But where does this come from? How do we know that these are the particles forming all the matter around us? Well, it all boils down to one simple observation: the Lagrangian¹ that describes the fundamental particles carries certain specific symmetries.

What are these symmetries? Well, there are several symmetries in the Lagrangian of the SM. Some of them are more obvious. For example, it must be symmetric under translations, which simply means that the physics of the SM one finds in a given point $\mathbf{r}$ must be the same if this point is translated to $\mathbf{r} + \mathbf{d}$. Translations are examples of global symmetries because this distance $\mathbf{d}$ is not a function of space-time coordinates. These are, of course, important symmetries. However, they are not enough to build the SM.

The SM Lagrangian also presents certain so-called *gauge* symmetries. Unlike the *global* symmetries, which represent invariance under *global* operations (e.g., translation), *gauge* symmetries represent invariance under *local* operations. In other words, the gauge operations depend on the space-time coordinates. The first example of gauge symmetries we usually encounter when studying physics is in electromagnetism. In that case, one could write the electric and magnetic fields generated by some charge distribution in terms of a scalar potential V and a vector potential $\mathbf{A}$. However, these potentials are not uniquely defined and, in fact, the same electromagnetic fields are generated when the potentials are transformed as $\mathbf{A} \rightarrow \mathbf{A} + \nabla\theta(t, \mathbf{x})$ and $V \rightarrow V + \partial\theta(t, \mathbf{x})/\partial t$, where $\theta(t, \mathbf{x})$ is some function of the space-time coordinates. This is an example of a gauge transformation and,

*English translation: “Nothing oppresses the heart like symmetry. It is because symmetry is ennui, and ennui is at the very foundation of grief. (...) Something more terrible than a hell where one suffers may be imagined, and that is a hell where one is bored.”

¹The Lagrangian of a system is a function of its degrees of freedom that is used to derive the equations of movement that describe the dynamics of that system.

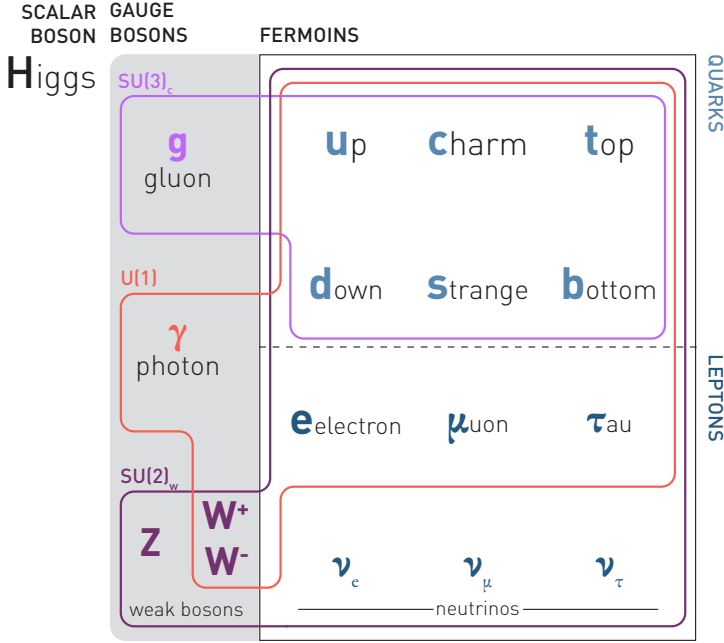


Figure 1: The particle content of the Standard Model of Particle Physics. Image produced in collaboration with Nicolas Le Roux.

therefore, this means that the Maxwell equations are symmetric under this specific gauge transformation.

Now, this is valid for classical electromagnetism. However, once quantum mechanics and relativity are taken into account, the classical theory of electromagnetism is cast in the formulation of Quantum Field Theory (QFT). When this is done, the potentials are combined into a *four-vector field*, $A_\mu = (V, \mathbf{A})$, representing the photon. At the same time, the charges that served as sources for the electromagnetic fields are now also represented by fields, $\Psi(x)$, which represent the electrically charged fermions in Fig. 1. In the QFT formulation, the Lagrangian is written in terms of those fields and the gauge transformation mentioned above now corresponds to taking $A_\mu \rightarrow A_\mu + \partial_\mu \theta(x)$ and, at the same time, $\Psi \rightarrow e^{i\theta(x)} \Psi$. These operations correspond to a $U(1)$ gauge transformation and the terms added to the Lagrangian by them cancel out, keeping the Lagrangian unchanged. This is what is meant by the statement that the Lagrangian contains a $U(1)$ gauge symmetry. In fact, the simple observation that the SM Lagrangian must be symmetric under $U(1)$ transformations is enough to introduce all the dynamics between electrically charged fermions and photons that, at the classical level, produce what we know of as electromagnetism, one of the three fundamental interactions of the SM. Analogously, the other two

fundamental interactions are also connected to the presence of gauge symmetries: the weak interaction is due to the $SU(2)_W$ symmetry and involves fermions carrying a charge called weak isospin; as for the $SU(3)_c$ symmetry, it involves fermions carrying the so-called color charge and accounts for the strong interaction. Just as the $U(1)$ has the photon, the other gauge symmetries also have their own *gauge bosons*².

This discussion is simply an overview of the SM, and the theory in its full complexity carries nuances that are out of the scope of this thesis³. However, it is interesting to note that this complex theory that can describe the dynamics of all the visible matter in the Universe arises from the simple statement that the Lagrangian should be invariant under the $U(1) \times SU(2)_W \times SU(3)_c$ gauge symmetries. This picture of the SM can be built due to the Noether theorem, which states that any continuous symmetry present in a Lagrangian carries a corresponding conserved charge. That is why, for each symmetry, I have explicitly mentioned which charges are involved in the corresponding interaction. In other words, the Noether theorem links a given interaction, due to a gauge symmetry, to a corresponding conserved charge. This way, the SM can be viewed as the matter forming fields, the fermions, interacting with each other via the three fundamental interactions, which are mediated by the corresponding gauge bosons exchanged between particles carrying the corresponding charges. The three interactions are represented in Fig. 1 by the different color outlines containing the particles that participate in the given interaction. For example, the pink outline indicates the particles participating in the strong interaction. The gluons are the mediators of that interaction, and they can be exchanged by quarks, which are the fermions that carry color charge. Since this is the interaction responsible for the phenomenology which is the focus of this thesis, we discuss it in a bit more detail next.

1.1 Quantum Chromodynamics

Quantum Chromodynamics (QCD) is the QFT that describes the dynamics of the strong interactions arising from the $SU(3)_c$ gauge symmetry. As mentioned earlier, this is the interaction mediated by the gluons and experienced by the particles that carry color charge. Unlike the well-known electric charge, that corresponds to one single value, the color charge can have three different values: red, green or blue. These are simply names and do not correspond to actual colors, but the analogy works because, just as the three colors together “cancel” out to form white, the three types of color charge sum up to the neutral

² $U(1)$ and $SU(N)$ are *symmetry groups* containing all the possible gauge transformations of the respective type. However, a group is defined by a set of rules and, if other entities obey the same set of rules of a given group they are said to form a *representation* of that group. For example, the gauge fields form one such representation, the so-called adjoint representation, whereas the fields of the Standard Model fermions form another one, the fundamental representation. Since the fundamental representation of the $U(1)$ group has dimension 1, the electromagnetic interaction “sees” the fermions as singlets and acts on each fermion field isolated. On the other hand, the fundamental representation of the $SU(N)$ group is N -dimensional. Therefore, those interactions involve N -plets of fermion fields $\Psi = (\Psi_1, \dots, \Psi_N)$

³For example, the weak and electromagnetic interactions are actually unified in the so-called electroweak interaction, due to the $SU(2)_W \times U(1)_Y$ symmetry which gets broken into the electromagnetic $U(1)$ symmetry we were discussing before via the Higgs mechanism. This process is far out of the scope of this text but I mention it here since it involves the Higgs boson shown in Fig. 1 and famously discovered in 2012 at the Large Hadron Collider.

color charge. However, this is not the only way to form a color neutral structure out of color charges. Just as the electric charge can be neutralized by its anti charge (e.g., an electron with charge -1 binds to a nucleus with charge $+1$ to form an electrically neutral atom) each of the color charges can be neutralized by the corresponding anti-charge. This means that each of the six quarks depicted in Fig. 1 can have one of the three types of color and each quark has a corresponding anti-quark carrying the anti-color. These particles combine to form color neutral structures named hadrons, which can be either (anti-)baryons, formed by three (anti-)quarks of each of the different (anti-)colors, or mesons, composed of a quark and an anti-quark.

The hadrons are the only possible composite structures of quarks that exist. Unlike electric charges, which can form stable charged structures such as ions, it is not possible to have a long-lived free particle with color charge. The reason for that lies in the very nature of QCD. Remember from the earlier discussion that electromagnetism is based on the $U(1)$ gauge symmetry whereas QCD arises from the $SU(3)_c$ symmetry. The $U(1)$ symmetry is an example of an *Abelian* symmetry, whereas $SU(3)_c$ is *non-Abelian*. This means that the order in which two $U(1)$ transformations are applied does not matter, whereas two $SU(3)_c$ transformations can give rise to different overall transformations depending on the order in which one applies them. This difference may sound simple, but it has one striking consequence: unlike the photons, which carry no electric charge, the gluons do carry color charge. Therefore, besides mediating interactions between two quarks, they can also interact among themselves, while the photon cannot interact with other photons.

Now, to understand how this changes the dynamics of the strong interaction when compared to electromagnetism, it is important to understand that another consequence of writing the Standard Model as a Quantum Field Theory is that the vacuum is not actually empty, but it is made of a superposition of quantum fluctuations⁴. However, in the presence of a charge, the quantum fluctuations of the vacuum will not be completely unpolarized. For example an electron-positron pair⁵ that emerges from the vacuum in the presence of an electron will be oriented such that the positron is closest to the electron. As a consequence, the electron's charge is effectively screened. In QCD, due to the gluon fields carrying color charge themselves, this process causes the opposite effect and a color charge becomes anti-screened by vacuum fluctuations. These particles that arise from vacuum fluctuations and thus must be short-lived are commonly referred to as virtual particles or "off-shell", as they are off the energy shell defined by four-momentum conservation. In specific circumstances that "fix" the energy-momentum conservation⁶, such particles can "come on-shell", namely, become physical particles, which can be observed in experiments for example.

Since such virtual particles are short-lived and cannot be directly observed, the only effect due to their presence is in the process of (anti-)screening of physical charges. Therefore, their effect can be taken into account by a change in the strength of an interaction. For

⁴The uncertainty principle allows for the appearance of particles out of the vacuum as long as they are short-lived enough.

⁵The uncertainty principle may allow particles to be created out of the vacuum, but it does not allow for the breaking of charge conservation.

⁶For example, an external particle can take or give any extra energy or momentum necessary to complete the four-momentum conservation by interacting with the off-shell particle.

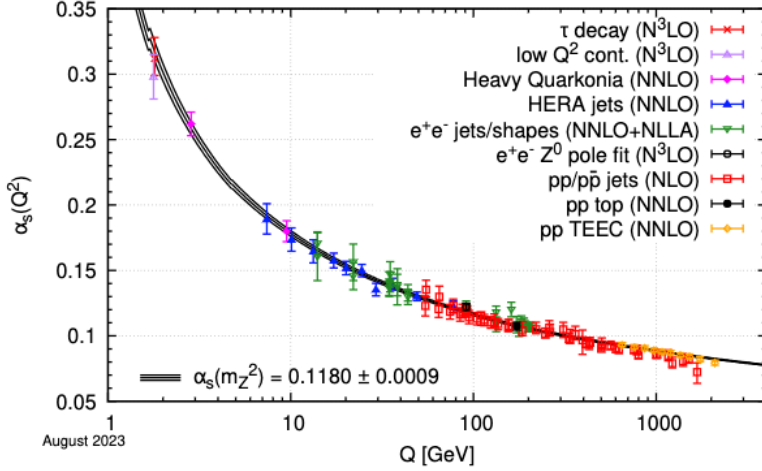


Figure 2: Running of the strong coupling calculated within the framework of QCD against experimentally measured values [1].

example, in electromagnetism, the strength of the interaction is characterized by the so-called “electromagnetic coupling”, α_{EM} . If we probe an electric charge from far away, for example by placing another electric charge there and measuring the strength of their interaction, the amount of quantum fluctuations screening the initial charge will be very large. Thus, the coupling between the two test particles will be more screened than if we had placed them closer together. In other words, the observed effect is that the electromagnetic coupling increases as the distance between two charges decreases. Now, the distance at which we can probe particles is inversely proportional to the energy of the “microscope” we use. In particle physics, the microscopes we commonly use are particle colliders. The higher the energy at which the particles are collided, the more “detailed” is the structure we can see, i.e., the closer is the distance between the charges we can probe. Therefore, as we increase the energy at which we probe some process involving electromagnetic charges, the electromagnetic coupling is observed to be larger and larger. In practice, α_{EM} actually does not increase very quickly with energy, and it can often be treated as a constant. This is not the case for the strong coupling.

Analogously to α_{EM} , the strong interaction is characterized by the strong coupling, α_S . The consequence of the gluons carrying color charge is that the strong coupling “runs” (changes) much more with energy compared to the electromagnetic one. However, the most striking difference is that it actually *decreases* with the energy of the process being probed. Fig. 2 shows this dependence as calculated from QCD compared to the experimentally measured values of α_S . Notice how quickly the strong coupling increases when the energy Q of a given process decreases (i.e., the distance increases). The plot is actually cut before 1 GeV, which is the typical energy of a hadron, but it continues increasing faster and faster. This means that it quickly becomes larger than 1, which is about three orders of magnitude larger than the electromagnetic coupling. But the greatest consequence of

the coupling reaching this value is the breaking of *perturbation theory* (PT).

Perturbation Theory

The details of how PT theory works will be left out of this text, although they can be found in many physics textbooks, not only within particle physics. However, it is important to understand that PT allows for the calculation of observables that cannot be otherwise computed by expanding them in a series. For example, the function $f(x) = \alpha/x$, where α is some constant, is not well-behaved when $x \rightarrow 0$. Therefore, if an observable has this functional dependence with some quantity x , it cannot be calculated in this limit. However, this function can be written in a series expansion as $f(x) = \sum_{n=0}^{\infty} (-\alpha)^n (x-1)^n$, which can be calculated for $x \rightarrow 0$, although it still has the issue of involving infinitely many terms. Nonetheless, if $\alpha < 1$, each term containing a higher order of α , that is, a larger power n , will contribute less than the previous one and the series can safely be truncated. Using this principle, PT can be used to calculate observables that, otherwise, are not well-behaved. If one wishes to reach higher and higher precision, one may compute higher order terms in the perturbative series.

All the calculations done in QFT are based on PT, including the one shown in Fig. 2. In that case the perturbative parameter α is taken to be α_S . When it becomes larger than 1, the terms of higher order in α_S actually contribute more and more to the final result and, therefore, PT can no longer help⁷. In any case, Fig. 2 shows that there are two different regimes characteristic of QCD: a perturbative one, where the coupling is small enough that PT can be used (the large Q tail of the plot), and a non-perturbative one for small values of Q , where perturbation theory breaks and one must resort to phenomenological models. The former is known as the “asymptotic freedom” regime, and the corresponding physical picture is one where quarks and gluons interact so weakly that they can be described as quasi-free particles; as for the latter, it corresponds to the “confinement” regime, when the strong coupling becomes so large that it is impossible to think of quarks and gluons as free particles, and they must be confined in hadronic structures. The characteristic scale at which confinement takes place is commonly referred to as Λ_{QCD} and its value is around 200 MeV.

This is the reason why quarks and gluons cannot be found as free particles at the typical energy scales we are used to. Therefore, if one wishes to study the QCD degrees of freedom, one must subject particles to extremely high energy scales, where asymptotic freedom can take place. One way to achieve that is at hadron colliders, where hadrons traveling at almost the speed of light collide with each other, allowing for processes involving asymptotically free quarks and gluons. However, it should be noted that these cannot be directly

⁷In practice, these “terms” correspond to Feynman diagrams. These diagrams describe the process of interest. Different diagrams can contribute to the same overall process via different intermediate states. The probability for a given process in QFT can be calculated by drawing all the corresponding diagrams. Feynman rules are then used to turn these diagrams into the correct mathematical expression for such probabilities. All the diagrams contributing to a given process must be computed in order to come up with the correct probability. However, the different diagrams may correspond to different orders in the perturbative series and, therefore, many of them can be “discarded” when the series is truncated to some order.

detected since they will be subjected to confinement by the time they reach the detectors. Additionally, one can collide the nuclei of heavy atoms, i.e., heavy ions. In this case, not only the energies are so large that asymptotic freedom takes place, but the free quarks and gluons that are created are in such a high density environment that they interact with each other via the strong force and form a state of matter that cannot exist in any other conditions. This and other aspects of heavy ion phenomenology will be discussed in the next section.

2 Heavy Ion Collisions

*Toutes les situations extrêmes ont leurs éclairs qui tantôt nous aveuglent, tantôt nous illuminent.**

— Victor Hugo, *Les Misérables*

In the previous chapter, we saw that the confinement property of QCD requires that, at the typical energy scales of the current state of the Universe, quarks and gluons remain bound into hadronic structures. Nonetheless, this has not always been the case and, a few microseconds after the Big Bang, the temperature of the Universe was actually above Λ_{QCD} [2]. This means that there was a point during the history of the Universe when the QCD degrees of freedom were asymptotically free. That is, of course, not currently the case. Nonetheless, it is possible to achieve the necessary conditions for asymptotic freedom by subjecting matter to extreme conditions of temperature and density, such as in the core of extremely dense stars [3] or by colliding the nuclei of heavy atoms at relativistic speeds. The latter is the focus of this thesis.

Fig. 3 shows a pictorial timeline of a typical heavy ion collision. As the highly Lorentz contracted ions pass through each other, an abundance of soft (low transverse momentum transfer) interactions between the nucleons happen. As a result, a large amount of the energy from the nuclei is deposited in the region where the collision took place and the nuclei remnants continue onwards (Fig. 3 b and c). Due to Lorentz contraction, all this energy is deposited in a very small volume and, thus, the energy density is extremely large. In fact, decades before the actual experiments took place, estimates showed that the energy density in the early stages of heavy ion collisions could reach up to 20 times the energy density of a typical hadron [4]. More recently, measurements have shown that, in central heavy ion collisions, the average transverse energy at midrapidity⁸ can be $\langle dE_{\perp}/d\eta \rangle \sim 1700$ GeV [5], thus compatible with the estimates. Therefore, at this point, the quarks and gluons making up the nucleons inside the nuclei behave as asymptotically free particles. However, they still interact strongly in a highly dense environment thus creating long range correlations

*English translation: “All extreme situations have their flashes that sometimes blind us, sometimes illuminate us.”

⁸The particle’s rapidity is related to the polar angle (away from the collision axis): $y = \frac{1}{2} \ln \left(\frac{1+\beta}{1-\beta} \right) \approx -\ln(\tan(\theta/2)) \equiv \eta$, where the approximation is valid for massless particles and, in that case, the rapidity, y , approaches the pseudo-rapidity, η . In this context, midrapidity refers to the central region around $y = 0$ (typically $|\eta| < 0.5$).

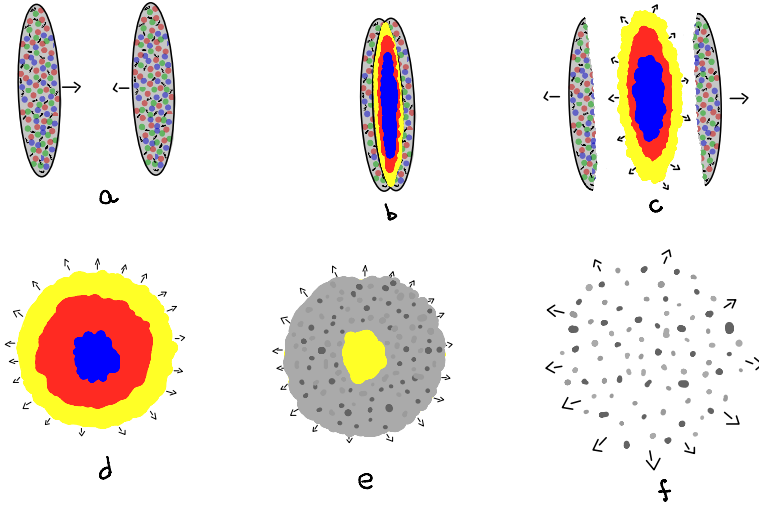


Figure 3: Pictorial timeline of a heavy ion collision: Two ions in the incoming beams collide (a); the multiple nucleon-nucleon interactions that take place deposit a large amount of energy within a Lorentz contracted region of space (b); this high energy density environment gives rise to a medium of strongly interacting particles (c); the medium hydrodynamically expands and cools down (d); when confinement temperature is reached, the partons hadronize back into colorless hadrons that may continue to interact in a dense hadronic gas (e); as this gas expands the hadronic interactions cease and the particles stream freely (f).

between them. As a result, these particles form a collective medium that can be well described by relativistic hydrodynamics [6]. This fluid of quarks and gluons then expands and cools down (Fig. 3 d) until it reaches the hadronization scale and confinement takes place once again (Fig. 3 e and f).

The existence of a medium formed by color charged particles when ordinary matter is subjected to extreme conditions of temperature and density was suggested a long time ago [4, 7, 8]. Nonetheless, the confinement property of QCD poses a challenge for the experimental confirmation of this medium's existence. Since it is not possible to directly detect quarks and gluons, one must identify signatures of this deconfined phase left over in the hadronic aftermath. Now, as mentioned before, most of the nucleon-nucleon interactions happening as the nuclei collide are soft with possibly few hard interactions taking place. The bulk of the QGP will be made of the outgoing particles from the abundance of soft interactions, whereas, the products of the hard interactions, which carry large transverse momentum, can quickly escape the medium, even if, at times, interacting with it. Therefore, one can think of two different classes of probes for this new state of matter:

soft probes, involving the outgoing particles from the multiple soft nucleon-nucleon interactions; and hard probes, formed by the particles originating in the more rare hard nucleon-nucleon interactions at the early stages of the collision, when the energy availability is at the peak. One example of the former is the observation of a near side ridge in the $\Delta\phi - \Delta\eta$ plane of the soft particle correlations [9]. This showed the presence of correlations between particles very far apart in rapidity, thus indicating that they must have originated at early times. Alternatively, the correlations of soft particles in the azimuthal plane work as a probe for the geometry of the initial colliding system, as will be discussed later. As for the remnants of hard scatterings, despite quickly escaping the collision region, they may still interact with the medium, thus both getting modified by it and, as more recently observed [10], modifying it in return.

A plethora of such signatures has been observed and used to confirm the existence of the QGP as well as to study its properties [2]. In the past decades, it was shown that the QGP has the smallest viscosity of any fluid known and thus behaves as an almost perfect liquid [2]. The evolution of such medium created in collisions of heavy ions could be very well described by relativistic hydrodynamics [6], which allows for the description of many of the signatures proposed for the QGP. In the following sections, two central probes of heavy ion collisions to the work developed in this thesis are discussed.

2.1 Jets as probes of a medium

Details regarding the process of formation of jets will be discussed in section 3.1. At the moment, it suffices to say that jets are collimated sprays of particles that are formed when partons undergo a hard scattering. If this scattering happens in the presence of a medium, the outgoing highly energetic particles will interact with the medium particles and will tend to thermalize. However, if this parton is energetic enough, it will escape the medium before thermalization actually happens, although not intact. Therefore, the jet formed in this manner will be modified with respect to a jet that would have evolved in vacuum and, thus, can carry signatures of the medium that modified it. As a result, jets can be used as probes for the medium of color particles produced in heavy ion collisions.

One way to use jets as probes of the medium, is to compare the population of jets observed in heavy ion collisions to that observed in proton-proton collisions, assuming, of course, that proton-proton collisions form a system that is too dilute⁹ to create a medium. This defines one very common class of observables: the nuclear modification factors, commonly referred to as R_{AA} and defined as:

$$R_{AA}^Q(p_\perp) = \frac{dN_{AA}^Q/dp_\perp}{\langle N_{\text{coll}} \rangle dN_{pp}^Q/dp_\perp}, \quad (2.1)$$

⁹Recall from earlier in this section that, while the energy at mid-rapidity in heavy ion collisions can get to $\langle dE_\perp/d\eta \rangle \sim 1700$ GeV, in proton-proton collisions that number is about three orders of magnitude below that even at the top LHC energies [11]. Therefore, in this sense, proton-proton collisions form systems that are much more dilute than heavy ion collisions.

where $\langle N_{\text{coll}} \rangle$ is the average number of binary pp collisions happening in the given class of AA collisions in consideration. The R_{AA} is the ratio of the yield of some quantity Q ($dN_{\text{AA}}^Q/dp_{\perp}$, for example, jets for $Q = J$) in heavy ion collisions to the yield in pp collisions ($dN_{\text{pp}}^Q/dp_{\perp}$) scaled by $\langle N_{\text{coll}} \rangle$. That is because, if there are no final state interactions with a medium in heavy ion collisions, it is expected that they will simply resemble an overlap of $\langle N_{\text{coll}} \rangle$ pp collisions¹⁰ and $R_{\text{AA}} = 1$. On the other hand, if the presence of a medium affects the yield of a given observable, then R_{AA} will not be equal to 1.

Glauber model

Notice that it is not possible to directly measure the number of binary collisions in a given heavy ion event. Therefore, Glauber modeling is a crucial phenomenological tool to precisely estimate $\langle N_{\text{coll}} \rangle$. They take as inputs the matter density profile inside a nucleus of a given species and a model for the cross section for interaction between two nucleons. With that, one can calculate the thickness of the overlap region between nuclei A and B at impact parameter $\mathbf{b}$ (the distance between the center of the nuclei in the transverse plane to the beam axis) as [12]:

$$T(\mathbf{b}) = \int T_A(\mathbf{s})T_B(\mathbf{s} - \mathbf{b})d^2s, \quad (2.2)$$

where $T_{A/B}(\mathbf{s})$ is the integral along the collision axis of the density profile of nucleus A/B at a distance $\mathbf{s}$ from the center. With that, for a given impact parameter $\mathbf{b}$, the probability that n binary collisions will occur is:

$$P(n, \mathbf{b}) = \binom{A}{B} [T(\mathbf{b})\sigma_{NN}]^n [1 - T(\mathbf{b})\sigma_{NN}]^{AB-n}. \quad (2.3)$$

Alternatively, one could take the matter distribution and the cross-section and use Monte Carlo methods to actually sample the number of binary collisions taking place over several events. More details on that will be discussed in Section 3.2.

Fig. 4 shows the observed R_{AA} in Pb+Pb collisions measured by the ATLAS experiment. The plot shows a remarkable suppression of jets. Notice that, even for very hard jets, up to 900 GeV, there is a substantial suppression taking place. Notice also that there are two classes of events shown in the figure: 0-10% and 30-40%. This refers to the centrality of the collisions, i.e., the smaller the percentage, the shorter is the impact parameter between the ions and, thus, the larger is the overlap region between them. Therefore, what this shows is that, when there is a large overlap, and thus more nucleon-nucleon interactions, the jet suppression is even more significant, pointing to the fact that, the more QGP is formed, the more modification the jets suffer.

To understand why this suppression happens, let us go back to the picture of a parton that acquired a large transverse momentum in a hard scattering. This parton will, then, emit Brehmsstrahlung radiation and, at the detector level, the resulting hadrons should be reclustered into a jet that will (hopefully) reflect the kinematics of the original hard parton. However, if the parton showering happens inside a medium, a particle emitted in the jet

¹⁰Or at least it will be close to 1 since there are other nuclear effects that can contribute.

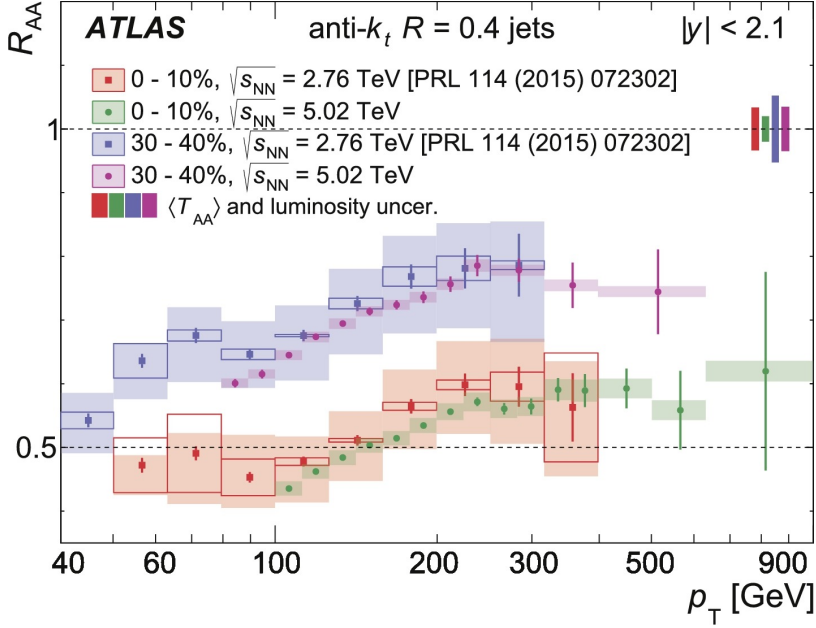


Figure 4: Observed values of jet R_{AA} by the ATLAS collaboration as a function of jet $p_{\perp}$ [13].

branching process may scatter elastically, if the coupling is weak enough, and thus lose energy and momentum to the medium particles. At the same time, an inelastic interaction with a medium particle will induce further Brehmsstrahlung radiation, which may also carry energy and momentum away from the jet. In fact, the latter is the driving factor of jet energy loss. As a result, one should expect that, if jets evolve inside a medium, they will be depleted of trasverse momentum when compared to jets that evolved in vacuum and, thus, the ratio in equation (2.1) will be less than 1. This is known as jet quenching.

Besides looking at their yield at a given $p_{\perp}$, there are other ways to study the medium by using jets. For example, one could look into events where a jet is created back to back with a Z^0 boson, which carries no color and, therefore, does not interact with the QGP. Therefore, using momentum conservation one can count on the boson's momentum as a reference and, this way, it is possible to probe the energy loss of jets without relying on having a true vacuum baseline [14, 15]. One may also search for changes to the shape of jets due to the presence of a medium with, for example, searches for jet broadening [16] or di-jet asymmetry [17], which show that jets are largely modified by the medium. Moreover, recent developments have allowed for the study of the space-time structure of jets in vacuum. With these new tools, it is possible to study the substructure of jets via energy correlators [18] or the formation time of jets [19] for example. These observables, therefore, are promising candidates for new ways to probe the medium [20] and its evolution. In fact, the modification of formation time of jets was the object of study of paper III in this thesis. This work provided not only insights to the possibility of studying the temporal structure

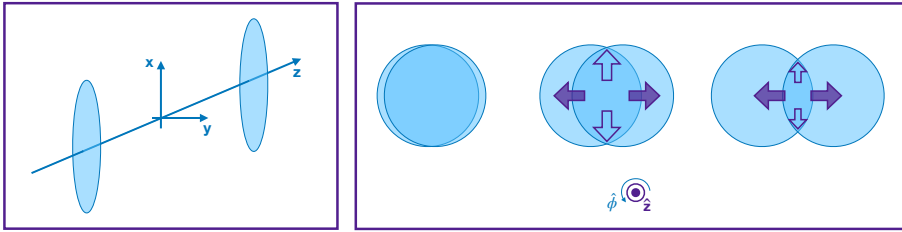


Figure 5: Left: definition of the collision axis along the direction connecting the incoming ions; right: different overlapping region geometries caused by different impact parameters.

of jets, but it also shed light on another form of modification of jets: the breaking of color coherence, which was further studied in paper IV. More details on that will be discussed in section 3.1.

2.2 Collectivity

In this section, we move away from hard probes and look at a phenomenon happening at soft energy scales. As mentioned earlier, the vast majority of the nucleon-nucleon interactions in heavy ion collisions will happen with a small momentum transfer. This creates a bulk of soft particles that interact strongly to form the hydrodynamic QCD medium. That means that these particles behave in a collective manner by interacting via the strong force and, therefore, the presence of collectivity may signal the formation of the fluid. Now, due to momentum conservation, once these soft particles hadronize, they will not dramatically change direction. Therefore, the distribution of soft hadrons in a given heavy ion collision event can give information regarding the fluid and how it expanded before confinement kicked in.

As an example, it is useful to think of the azimuthal distribution of particles. For this, we define the azimuthal angle as the one going around the beam axis on a plane transverse to it, i.e., the xy plane in the left most sketch in Fig. 5. The initial state of a given collision is rotationally invariant. Therefore, the final state will also reflect such symmetry unless it gets broken by some mechanism. In other words, over several *independent* nucleon-nucleon collisions, the azimuthal distribution of final state particles is completely flat. On the other hand, if the post collision environment is dense enough that the particles interact and form a medium, their momentum distribution will show correlations (other than the one due to momentum conservation or hadronic rescattering for example).

The three sketches on the right side of Fig. 5 show the instant of the collision in three different cases as seen from the beam axis. In the first of those sketches, the overlap between

the ions is almost complete and, therefore, the overlap region is isotropic, as are the ions. However, in the other two cases, the overlap region shows an anisotropy. Therefore, when a fluid is formed in this non-isotropic region, the particles flowing away hydrodynamically will push against each other and build up pressure gradients. These gradients will be larger in the direction of the short axis of this approximately elliptical region (the filled arrows in the right-hand side of Fig. 5) and will transform the spatial anisotropy into a momentum-space anisotropy. Therefore, in the momentum distribution of the soft particles in this event, there will be an enhancement of momentum in the direction of the filled arrows of Fig. 5 and a depletion in the direction of the empty arrows. Moreover, this difference will depend on the impact parameter between the nuclei. To quantify the azimuthal anisotropy, the particle distribution can be described as a Fourier series:

$$\frac{dN}{d\phi} \propto \frac{1}{2\pi} \left(1 + 2 \sum_n v_n \cos(n[\phi - \Psi_n]) \right), \quad (2.4)$$

where the v_n coefficients are known as flow coefficients of order n , which quantify the contribution from the n^{th} harmonics; and Ψ_n is the azimuthal angle of the symmetry axis of the n^{th} harmonic. As an example, for $n = 2$, Ψ_2 corresponds to the angle of the short axis of the ellipse that best describes the distribution and v_2 , thus, characterizes the ellipticity of the distribution. Therefore, v_2 is commonly called the *elliptic flow*.

It should be emphasized that the mechanism described above can only affect the low- $p_\perp$ particles coming from soft nucleon-nucleon interactions and forming the QCD medium. This is because the high- $p_\perp$ particles created in the hard scatterings in the early stages of the collision quickly escape the medium and do not fully thermalize. Therefore, they are not subjected to flow effects. As a result, any sign of a v_2 in particles of high- $p_\perp$ must have another origin. From the discussion in the previous subsection, it was clear that high momentum partons can lose energy to the medium even if they do not fully thermalize. On the other hand, we just saw that, depending on the impact parameters between the ions, there is a spatial anisotropy in the medium. Therefore, a hard parton with momentum along the empty arrows in Fig. 5 will take longer to escape the medium compared to a particle traveling along the short axis (filled arrows) of this ellipse. Accordingly, the suppression of jets will be anisotropic in ϕ . In other words, high- $p_\perp$ particles may acquire azimuthal anisotropies via path-length dependent energy loss. Fig. 6 shows the v_2 values observed by the CMS collaboration in Pb+Pb collisions at different centralities as a function of $p_\perp$. It is clear that the low $p_\perp$ particles show very large anisotropy, especially at more peripheral events, where the overlap regions is expected to be more elliptical but, for the high $p_\perp$ ones, there can still be a substantial v_2 , indicating that there is indeed a path-length dependence in the energy loss of particles.

Using these and other observables, it was determined that droplets of a Quark Gluon Plasma are created in heavy ion collisions [22–24]. This fluid was studied and characterized as an almost perfect liquid, as mentioned earlier in this section. The formation of such material is enabled by the extremely high densities to which this system is subjected. This scenario is contrasted to that of pp collisions, where it is assumed that there are no

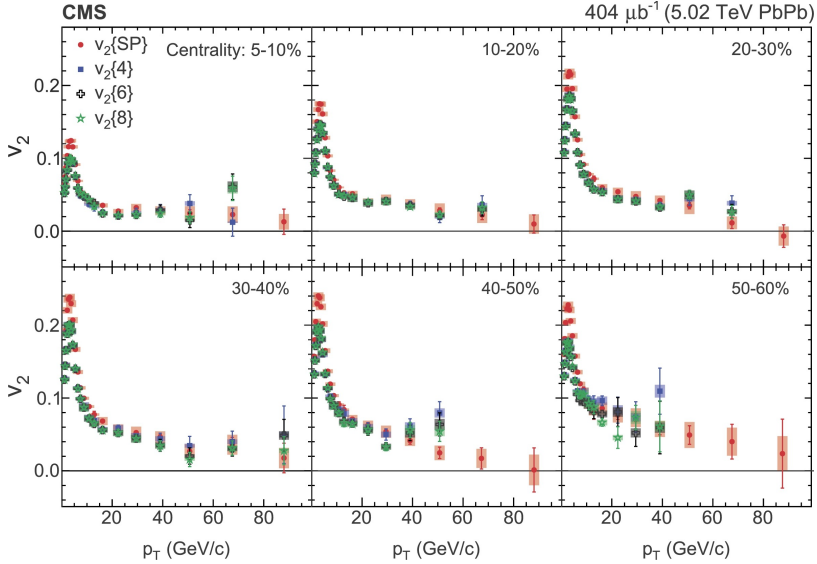


Figure 6: Results of v_2 using different measurement techniques by the CMS collaboration as a function of hadron $p_{\perp}$ for different centrality classes [21].

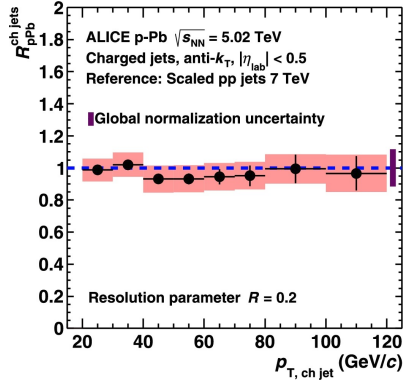
final state interactions whatsoever. Therefore, one might wonder what happens in between these two contrasting scenarios. Is there a sharp transition from no rescatterings to medium formation? At which point this transition happens or starts to happen? To address these questions, it is useful to look into what happens in small collision systems.

2.3 Small Systems

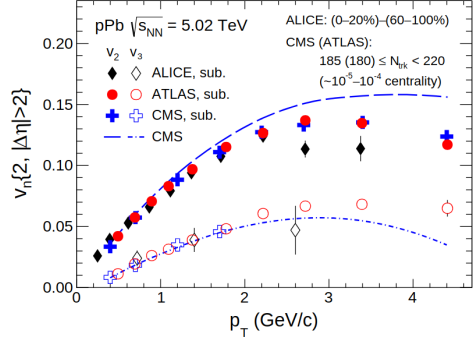
The panorama of heavy ion collisions discussed above is very different from the way proton-proton collisions are viewed. In these dilute systems, it is assumed that the products of a scattering propagate freely without interacting with each other. Even if multiple partons are allowed to scatter in a given pp collision, each of the scatterings are (almost) completely independent¹¹. On the other hand, when modelling relativistic heavy ion collisions, the formation of a collective medium of color particles flowing hydrodynamically is assumed [25]. The question then arises: how can these two contrasting pictures come together? At which point can one go from a “simple” picture of the jet evolution in vacuum (as will be discussed in section 3.1) to the complex collective behavior of hydrodynamics? To tackle these questions, it is worthwhile to look at what happens in collisions of smaller systems such as proton-ion or even at high multiplicity proton-proton collisions.

It is interesting, for example, to look into these small systems and search for medium signatures there. When this was done, it was quickly noted that jets do not significantly lose energy. Fig. 7a shows the R_{pA} (the analogous of R_{AA} , but for proton-ion (pA) collisions)

¹¹Apart from trivial correlations such as those due to conservation laws.



(a)



(b)

Figure 7: (a) Measurement of jet suppression as a function of $p_{\perp}$ by the ALICE collaboration in p+Pb and Pb+Pb collisions at different centralities [29]; (b) Observed values of v_2 and v_3 in pPb collisions as a function of $p_{\perp}$ [27].

obtained by the ALICE experiment in [26]. It is clear that the ratio is compatible with unity. On the other hand, Fig. 7b (reproduced from [27]) shows that signs of collectivity were actually observed in those systems by the ALICE collaboration. More surprisingly, this figure shows that, even particles with intermediate to high- $p_{\perp}$, present significant azimuthal anisotropy, which would indicate path length dependent energy loss. That is in apparent contradiction with the observation in Fig. 7a, which shows that jets do not suffer energy loss in pPb collisions. This matter was thoroughly studied and other signatures of collective behavior were observed in p+Pb and even in high multiplicity pp collisions. But, so far, no signs of jet quenching were observed in those systems [28].

This conundrum raises questions of how sensitive the usual QGP observables actually are to the presence of a medium. It also highlights the need for observables that are not dependent on a pp baseline. It pushes for a more thorough understanding of the dynamics of energy loss and the mechanisms, other than flow, that can build up anisotropies. This was the motivation for all the papers in this thesis: to understand how this phenomenology emerging from a high density QCD environment in heavy ion collisions can be reconciled with the observation of similar phenomena in dilute systems. The approach chosen to address these questions within the works in this thesis was to use computational methods. More specifically, we used Monte Carlo simulations and, therefore, we discuss those tools in more details in the next section.

3 Monte Carlo methods and QCD phenomenology

But you don't have to be able to swim to know a fish, you don't have to shine to recognise a star...

— Ursula Le Guin, *The Dispossessed*

Monte Carlo (MC) is a class of methods for numerical calculation based on sampling of pseudo-random¹² numbers [30]. Despite this stochastic structure of MC methods, they are tools for solving deterministic problems, such as finding the integral of mathematical functions for instance.

An intuitive example can be that of finding the area of a circle by randomly selecting points on a 2D surface of known area containing that circle. The area of the circle is, then, determined as the ratio of the number of points that happened to fall within the circle to the total number of points sampled. Of course such a result will always be an approximate one and, for this simple problem with a straightforward analytical solution, not the best one. However, this approximate solution has a well known error, which can be shown to scale as $1/\sqrt{N}$, where N is the number of random numbers sampled. That means that, by increasing the statistics, one can decrease the error and, although it may seem like it does not decrease fast enough, it has the great advantage of not depending on the number of dimensions in the integral. For comparison, the error obtained in the Simpson method, a common numerical integration tool, scales as $1/N^{4/d}$, where N is the number of numerical steps used for the calculation. That means that, for an 8 dimensional integral, the two methods already have comparable errors. And, although that might seem like a lot, it should be noted that, in the context of hadron colliders, we are interested in calculating cross-sections for processes of two hadrons interacting to yield N particles. This means that we must solve integrals which involve the final state four-momenta of each of the N particles and, therefore, these integrals can have up to $4N$ dimensions. Thus, for a process of two hadrons going to three final state particles, MC methods are already in advantage compared to the Simpson one. Besides that, MC methods also allow for the integration of functions with complicated integration limits, which are often the case in phase space integrals.

Therefore, it is clear that MC methods are extremely useful in computing the high dimensional integrals involved in hadron collision phenomena. However, the use of these methods in the field goes beyond solving integrals. Another common application of MC tools is sampling from probability distributions, which is extremely useful in simulating stochastic processes. For example, consider the expression for the integration of the cross-section for a process $ab \rightarrow cd$:

¹²Random numbers provided by computational algorithms used in MC calculations are never truly random, but can behave as random numbers as long as the correct conditions for the given algorithm are met. Such conditions can be, for example, keeping the number of sampled numbers below a certain threshold, which can be in the order of 10^{6000} in modern algorithms.

$$\sigma_{ab \rightarrow cd} = \int d\Phi_2 \frac{d\sigma(p_a p_b \rightarrow p_c p_d)}{d\Phi_2}, \quad (3.1)$$

where p_i is the four momentum of particle i and $d\Phi_2$ is the phase space for the 2-particle final state, i.e., an infinitesimal volume in energy-momentum. The integral over $d\Phi_2$ means that one should consider all possible points in energy-momentum space where the 2 particles can be created in order to compute the total cross-section for the $ab \rightarrow cd$ process. This is precisely the type of integral that one can calculate with MC by generating random phase space points and summing the value of the function to be integrated ($d\Phi_2 d\sigma(p_a p_b \rightarrow p_c p_d)/d\Phi_2$ in this case) at that phase space point¹³. On the other hand, if a phase space point is generated in the process for calculating such integral, and, since that point is a legitimate physically allowed point, this procedure can very well be used for simulating one of the paths via which this $2 \rightarrow 2$ process may happen. Now, the cross-section for a given process at a given phase-space point is directly related to the probability for this path to be taken. Therefore, one may proceed to generate several phase space points sampled by a probability related to the differential cross-section and actually simulate the production and propagation of the final state particles at that point. If this is done correctly, the integrated cross-section over the simulated final states will be the result of the integral in equation (3.1) with the added bonus that one will obtain pseudo-data very similar to the experimentally measured data, being able to apply to this simulated data the same cuts and constraints from the experiment of interest. And this is just one simple example, but, if one considers the full complexity and all the steps involved in hadronic collisions, it is clear how powerful MC methods are for testing theoretical formalisms against experimental data. Therefore, let us delve a bit deeper into the process of simulating hadronic collisions.

Fig. 8 depicts the different processes involved in the simulation of hadronic collisions: starting from two incoming hadron beams all the way to the N particle final state. This image is from the SHERPA [31] event generator, but it gives a good general overview of what other multipurpose event generators, such as PYTHIA [32] and HERWIG [33], do: make use of factorization theorems to separately treat processes at different energy scales thus generating N -particle final states according to the cross-section:

$$d\sigma_{hh \rightarrow N} = \mathcal{P}_{\text{beams} \rightarrow ab} \otimes d\sigma_{\text{hard process}} \otimes \mathcal{P}_{\text{QCD shower}} \otimes \mathcal{P}_{\text{hadronization}} \otimes \mathcal{P}_{\text{decays}} \otimes \mathcal{P}_{\text{QED emissions}} \otimes \mathcal{P}_{\text{MPI}}. \quad (3.2)$$

The right-hand side represents the factorization of the process at each of the different scales treated, with the colors (approximately) corresponding to the respective processes in Fig. 8.

Let us take a closer look at each of the factors starting with $\mathcal{P}_{\text{beams} \rightarrow ab}$: this is related to the probability for extracting partons a and b from each of the beams, i.e., the beams are

¹³That is the general idea of how to use random number generation to compute integrals in MC, but there are more robust and optimized methods derived from this.

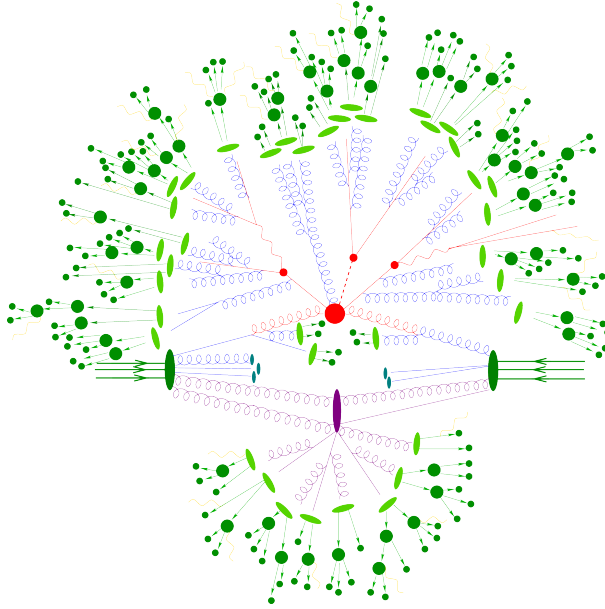


Figure 8: Schematic picture of a Monte Carlo event generation procedure [31]. The different colors refer to different energy scales. See text for a more detailed description.

described by probability density functions¹⁴ for the different possible partons as a function of the energy scale. Therefore, using MC methods, these functions can be sampled for a parton of a given type with a given four momentum fraction of the hadron.

The next¹⁵ step is to do the **hard scattering** between the two partons. For that, the matrix element(s) corresponding to the process(es) of interest is(are) sampled for a number of outgoing partons and their four momenta.

Those partons are then fed into a **QCD parton shower** where they will emit further Brehmsstrahlung radiation. However, note that the partons extracted from the beams in Fig. 8 also radiate. This is taken care of by the *initial state parton shower*, which does a backward evolution from the matrix element to the beam scales. As for the *final state parton shower* (to which the outgoing partons from the hard scattering are subjected), more details will be discussed in section 3.1. For now, it is enough to know that, as they radiate, their four momenta are split into more partons and the energy scale of the shower goes down. Since the parton shower relies on perturbative expansions, it will stop at some infra-red cutoff scale. At that scale, confinement binds the partons back into hadronic structures.

This is the point where **hadronization** takes place and, as a non-perturbative process, it relies on phenomenological models. There are very well motivated models that have had great

¹⁴A QCD motivated extension of the quark model allows for the description of the hadrons in terms of probability densities for the different types of partons, thus named the parton model. These densities can be measured in experiments to great accuracy.

¹⁵In practice, everything usually starts from the hard process and is evolved backwards into the beams.

success at describing experimental data. The most successful and widely spread of these models is the Lund string model [34] implemented in the PYTHIA event generator [32]. It models the color fields between partons moving away from each other¹⁶ as strings with certain tension that can break into more partons. The process goes on until the energy scales of the string are low enough that they cannot break anymore and the leftover partons are bound to each other in hadronic structures. Alternatively, a cluster hadronization model can be employed (e.g., SHERPA [31] and HERWIG [33]). In that case, at the end of the parton shower, the gluons are split into quark-anti-quark pairs and neighboring color charges are clustered into color singlet structures, which will decay until the scale of hadron masses is reached [35].

Therefore, after these steps, an ensemble of hadrons will be leftover. However, many of them are unstable. Therefore, they will **decay** into stable hadrons according to decay rates that can be measured in independent experiments. Again, MC methods can be used to simulate these decays according to the probabilities given by the decay rates.

The emission of **QED radiation** must also be taken into account. This can happen as Bremsstrahlung radiation being emitted off the quarks since they are electrically charged, but the hadron decay process also contributes substantially to the photon production¹⁷. Finally, recall that the incoming hadrons are extended objects composed of more than one parton. Therefore, it is possible that more than one pair of partons will scatter and undergo all the aforementioned processes. This is taken into account by **multiple parton interaction** (MPI) models.

3.1 Initial and final state parton showers

In this section, we focus on the blue lines pictured in Fig. 8. They represent the parton showers. Notice that there are blue lines coming from the incoming hadrons, but there are also blue lines that are coming from the final state partons created in the hard scattering process. These represent two seemingly different phenomena: the initial (space-like) and final (time-like) state parton showers. Although they seem different, they are represented by the same color because they stem from the same fundamental phenomenon: the emission of QCD radiation.

This phenomenon is analogous to the well known QED example of an electrically charged particle in motion: at high velocities, the electromagnetic fields around the charge get Lorentz boosted and become increasingly confined in the plane perpendicular to the direction of motion. This means that the electric and magnetic fields around the charge become orthogonal to each other. As a result, one can identify the energy stored in these classical fields as quanta of electromagnetic fields, namely, photons [35]. This picture is called the equivalent quanta because the continuous energy flux stored in the fields can be interpreted as an equivalent flux of quanta (the photons in this QED example).

¹⁶Remember from the discussion in section 1.1 that the strong coupling increases as the distance increases.

¹⁷Photon production at the level of the matrix element, is also possible. However, this is much less likely given the smallness of the QED coupling compared to the QCD one.

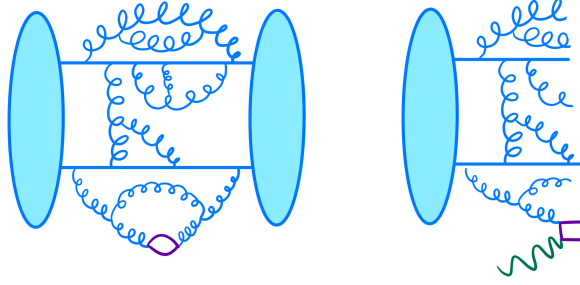


Figure 9: Left: a collection of partons in a completely coherent state with virtual fluctuations being continuously emitted and reabsorbed; right: a photon interacting with one of the virtual partons breaks the coherence of the state and virtual quanta come on shell.

Analogously, a color charge surrounded by its color fields can be interpreted as the charge accompanied by an equivalent flux of partons (quarks and gluons). Due to momentum conservation, these partons are off-shell and, considering the uncertainty principle, the lifetime of such quanta will be rather short. Therefore, when there is a highly boosted charge, it will be accompanied by a flux of quanta that will be continuously emitted and reabsorbed. This is precisely what happens when hadrons are accelerated in colliders and, this constant emission and reabsorption (imposed by momentum conservation and the uncertainty principle), guarantees the coherence of the quantum state, as illustrated in the left-hand side of Fig. 9. The right-hand side depicts what happens when an external field interacts with one of the virtual states in the quantum fluctuations: it may cause that state to go on-shell and become a long-lived physical particle, which will cause other virtual states to do the same.

Therefore, the incoming hadrons in a collision are constantly emitting and reabsorbing virtual states. As a result, if we want to know what happens when the hadrons actually collide, it is important to ask: at any given energy scale, what is the density of partons carrying a fraction x of the hadron's four momentum? The answer to this question is given by Deep Inelastic Scattering (DIS) experiments. In DIS, a highly virtual photon interacts with the constituents of the hadron. The virtuality of such photon, Q^2 , sets the resolution at which it probes the hadron. Using this as a “microscope” of resolution $1/Q^2$, it was shown that the hadron can be described by probability density functions (PDFs), which give the probability of finding a parton i in hadron h at scale Q^2 carrying fraction x of the hadron's four momentum¹⁸: $f_{i/h}(x, Q^2)$. Since the PDFs are non-perturbative objects, they cannot be calculated from first principles. Nonetheless, they can be measured at a given energy scale and given as input to evolution equations which, then, provide their value at another scale. These are the DGLAP evolution equations [35]:

¹⁸Details regarding the calculation of the DIS cross-section are out of the scope of this text and can be found in, e.g., Ref. [36].

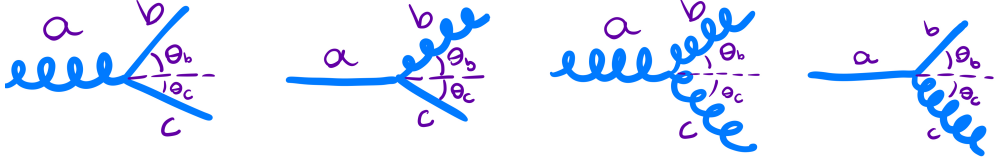


Figure 10: Leading order diagrams for the calculation of the four $a \rightarrow b + c$ QCD splitting functions in the kernel of equation (3.3).

$$\frac{\partial}{\partial \log Q^2} \begin{pmatrix} f_{q/h}(x, Q^2) \\ f_{g/h}(x, Q^2) \end{pmatrix} = \frac{\alpha_S(Q^2)}{2\pi} \int_x^1 \frac{dz}{z} \begin{pmatrix} \mathcal{P}_{qq}(\frac{x}{z}) & \mathcal{P}_{qg}(\frac{x}{z}) \\ \mathcal{P}_{gq}(\frac{x}{z}) & \mathcal{P}_{gg}(\frac{x}{z}) \end{pmatrix} \begin{pmatrix} f_{q/h}(z, Q^2) \\ f_{g/h}(z, Q^2) \end{pmatrix}, \quad (3.3)$$

where $\mathcal{P}_{ab}$ are the so-called splitting functions. They give the probability for the splitting $a \rightarrow bc$. The structure of the DGLAP equation is such that, the PDF for a parton i is enhanced by the probability of a splitting that produces that parton times the PDF of the parton that splits into i . The splitting functions are the kernels of the evolution equations for the PDFs and, to leading order, they can be calculated from diagrams such as those in Fig. 10. Moreover, it can be shown that these PDFs are process independent and, therefore, one can use the DIS measured PDFs to describe hadrons in other processes.

It is also important to notice that equation (3.3) is obtained within the *collinear factorization* picture. This is based on the observation that the matrix elements for parton emission off other partons show an enhancement at small angles. In this limit, it can be shown that [37]:

$$d\sigma_{n+1} = d\sigma_n \frac{dQ^2}{Q^2} dz \frac{\alpha_S}{2\pi} \hat{P}_{ba}(z), \quad (3.4)$$

where $\hat{P}_{ba}(z)$ are the regularized¹⁹ splitting functions. In other words, the DGLAP equation (3.3) can be interpreted as describing a process for producing $n + 1$ particles as the process for producing n particles plus one emission. This is done iteratively by means of the evolution in equation (3.3) from some hard scale to smaller scales. Going back to the picture of a charge surrounded by a flux of quanta, these emissions can be seen precisely as these quanta coming on shell due to the breaking of the coherence of the initial state when the hard scattering takes place. This is the origin of the initial state parton shower, the blue lines branching from the incoming hadrons in Fig. 8.

As for the final state parton shower, the blue lines branching from the outgoing partons from the hard scattering, it stems from the same phenomena as the initial state one. The difference is that there are no hadrons at this point in the collision process. Therefore, one

¹⁹The splitting functions show divergences in the limit of soft gluon emissions ($z \rightarrow 0$ or $z \rightarrow 1$). Therefore, one must regularize them before calculating cross sections. This is usually done using the plus prescription. More details can be found, e.g., in Refs. [35, 37, 38].

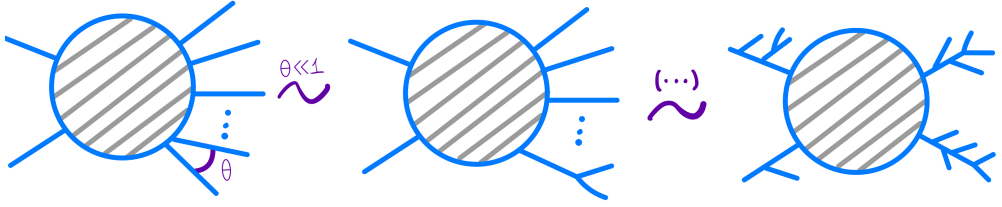


Figure 11: Depiction of the factorization of collinear emissions leading to the parton shower picture.

cannot talk about hadron PDFs. Nonetheless, the same evolution equations as (3.3) can be used to describe the final state emissions as long as the PDFs are replaced by *fragmentation functions*, $D_{p/h}(x, Q^2)$, which determine the probability for a parton p to give rise to hadron h at scale Q^2 . In this case, the evolution of the DGLAP equation is performed from the hard scale Q^2 down to the scale where perturbation theory breaks and hadronization takes place.

In conclusion, the calculation of the cross-section for a $2 \rightarrow n$ process would be extremely cumbersome (if not impossible). Fortunately, it may also be unnecessary, given that the matrix elements for these processes are largely enhanced in the limit in which two of these n partons are collinear, as shown in the left-most sketch of Fig. 11. Moreover, equation (3.4) shows that, in this limit, the cross-section can be factorized as that for the production of $n - 1$ particles and the splitting of one of those particles into two others. The same logic can be applied to the resulting diagram (middle sketch in Fig. 11) recursively until one obtains simply the cross-section for the $2 \rightarrow 2$ process in which the incoming and outgoing particles are subjected to parton showers (right-most sketch in Fig. 11). Although this is an approximation for the collinear limit, it captures the phenomenology of these processes rather well. Besides, unitarity can be used to estimate the effect of neglecting the finite contributions. However, another enhanced contribution that was not taken into account is that of the emission of soft gluons. Despite being soft, their presence has striking consequences on the QCD radiation pattern, which will be discussed in the following subsection.

3.1.1 Color coherence and angular ordering

In order to take into account the soft enhancements, one could start from the collinear factorization picture described before and add soft gluon emissions to the collinear splittings of Fig. 10. For example, in the $g \rightarrow q\bar{q}$ splitting, soft gluon emissions can be added to each of the two fermion legs as shown in the first row on the right-hand side of Fig. 12. Such emissions are of course enhanced when $\tilde{\theta} \rightarrow 0$, but they are also enhanced in the

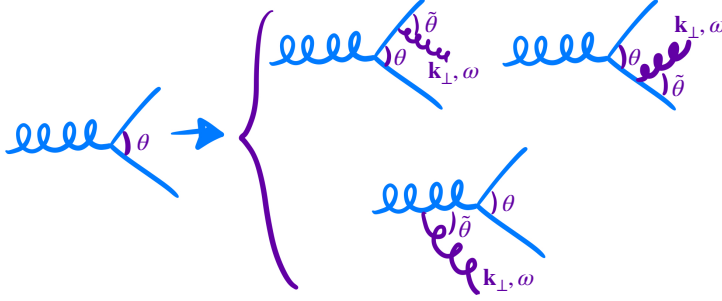


Figure 12: A soft gluon emission off one of the fermion lines after a $g \rightarrow q\bar{q}$ splitting. Color coherence requires that $\tilde{\theta} < \theta$. See text for more details.

limit where the gluon energy $\omega \rightarrow 0$. In the latter case the angle does not need to be small. However, if the angle is large compared to the angle between the quark and the anti-quark, would it make sense to differentiate the cases where the gluon is emitted from different fermion lines? In other words, can the gluon resolve the two partons?

To answer that question, let us start by noting that this soft gluon could very well be reabsorbed by the (anti-)quark. Therefore, we are interested in the case in which it has a lifetime long enough to be seen as a real emission and become, itself, an independent source of radiation. To estimate that lifetime, one can make use of the uncertainty principle, which leads to $t_f \sim 1/(\omega\tilde{\theta}^2)$ [35, 37, 39]. This is referred to as the *formation time* of a parton. After that time, the separation between the quark and the anti-quark is $\Delta b = t_f\theta$. On the other hand, the transverse wavelength of the emission is $\lambda_\perp \sim 1/k_\perp \sim 1/(\omega\tilde{\theta})$. Therefore, these two distance scales define the resolution criterion. If $\lambda_\perp > \Delta b$, then the gluon cannot resolve the two partons separately and it actually “sees” the two partons as a single *coherent* source. In other words, it couples to the splitting gluon, not to one of the fermion lines, as shown in the bottom row of Fig. 12.

This characteristic is known as *angular ordering* because it imposes the following relation on any two consecutive splittings²⁰:

$$\lambda_\perp < \Delta b \quad \Leftrightarrow \quad \frac{1}{\omega\tilde{\theta}} < \frac{\theta}{\omega\tilde{\theta}^2} \quad \Leftrightarrow \quad \tilde{\theta} < \theta. \quad (3.5)$$

In fact, this is also valid for QED. However, in that case, the soft gluon emission would

²⁰Alternatively to this phenomenological argument, angular ordering can be proved in a more formal way by calculating the amplitudes in the top right side of Fig. 12. The destructive interference between the two diagrams gives rise to angular ordering. The details of this calculation can be found in, e.g., [37].

be a soft photon emission and, if it were not able to resolve the charges individually, the electric charge of the system that the photon *actually* resolves would be zero. Since photons cannot couple to systems with zero electric charge, then this emission would be forbidden. In the case of QCD, however, the situation in which $\lambda_\perp$ is larger than Δb does not forbid the emission. However, the gluon, in that case, is effectively emitted coherently by the color dipole. Therefore, this coherent emission is a phenomenon exclusive of QCD and is, therefore, a phenomenon due to *color* coherence specifically.

Overall, what we learned is that, the main features of a general $2 \rightarrow n$ process in QCD are captured by the collinear splittings described by the DGLAP equation (3.3) satisfying the property of angular ordering. The result is a radiation spectrum given by [39]:

$$dw^{k \rightarrow l+m} = \frac{\alpha_S(k_\perp^2)}{4\pi} \frac{d^2 k_\perp}{k_\perp^2} dz P_{lk}(z), \quad (3.6)$$

with angular ordering being imposed at each consecutive splitting. In this equation, $P_{lk}(z)$ are the unregularized splitting functions for $k \rightarrow l + m$. Such divergences must be treated and, in Monte Carlo algorithms, this is often done by imposing a cutoff in $k_\perp$ above Λ_{QCD} , where perturbation theory should no longer apply and, thus, the parton shower, which is perturbative in nature, should no longer be used to describe the physical picture. With this, one can build Monte Carlo algorithms for the construction of a parton shower, as will be briefly discussed in the following subsection.

3.1.2 Monte Carlo parton showers

The process we want to simulate is that in which partons split stochastically into two other partons according to probabilities given by QCD. This resembles the process in which a radioactive nucleus with half life τ decays. If this nucleus is intact at $t = 0$, the probability that it has not decayed after some time Δt is: $e^{-\Delta t/\tau}$. A similar formulation can be written for the case of parton splittings. However, in light of the previous discussions, and so that a connection with the DGLAP equation (3.3) can be made, one should view the sequential parton splittings as ordered, not in time, but in the energy scale²¹, q^2 . With that, and making use of equation (3.6), the probability that parton k has *not* split between the scales Q_0^2 and Q^2 is given by the *Sudakov* form factor [35, 37, 40]:

$$\Delta_k(Q^2, Q_0^2) \equiv \exp \left(- \sum_l \int_{Q_0^2}^{Q^2} \frac{q^2}{dq^2} \int dz \frac{\alpha_S}{2\pi} P_{lk}(z) \right), \quad (3.7)$$

where the sum runs over all possible splittings $k \rightarrow l + m$. Since $\Delta_k(Q^2, Q_0^2)$ is the *no splitting* probability between scales Q_0^2 and Q^2 , then, the probability of no splitting between

²¹On the other hand, we have discussed how the consecutive splittings must be angular ordered. Therefore, one could make use of the relation $q^2 \sim z(1-z)\theta^2 Q^2$ to build a parton shower ordered in angle. Since the angle is also related to the transverse momentum, another choice of ordering variable can be $k_\perp$. [35, 40]

any two scales Q_1^2 and Q_2^2 is $\Delta_k(Q_1^2, Q_0^2)/\Delta_k(Q_2^2, Q_0^2)$. An MC algorithm can, then, make use of this to sample, using random number generators, the scale Q_2^2 at which a parton of invariant mass Q_1^2 will split. If this Q_2^2 is outside the boundaries of the evolution, i.e., below the infrared cutoff, it means the parton simply does not split. Once a splitting scale has been generated, the splitting functions $P_{lk}(z)$ can be used to sample a value for the momentum sharing, z , between the daughter partons. After that, the complete kinematics can be set and the daughter partons, which are in a lower (higher) scale in the space (time)-like parton shower, will then go through the same process until there are no more possible splittings [37]. Notice that, in this case, the unregularized splitting functions are used in equation (3.7). Therefore, in order to regularize the Sudakov factor, a cutoff must be chosen, i.e., $z < 1 - \epsilon(q^2)$. That is equivalent to saying that, if $1 - \epsilon(t) \leq z \leq 1$, the soft parton cannot be resolved. Therefore, Δ_k should in fact be interpreted as the no *resolvable* splitting probability.

This is a general view of how a parton shower can be constructed with MC algorithms. In practice, there are several nuances and details in the construction of such objects. One example is the choice of ordering variable. A few options have already been mentioned: one can use the splitting parton's virtuality as ordering variable, as implemented, for example, in PYTHIA 6 [41]; the splitting angle, e.g., HERWIG [33]; or the transverse momentum as done in PYTHIA 8 [32]. Note that, in the way the Sudakov factor is written in equation (3.7), the coherence effects discussed in the previous subsection are not accounted for. However, if transverse momentum or splitting angle are used as ordering variables, angular ordering is satisfied by construction. Otherwise, it has to be imposed on top of this as a splitting rejection criterion for example. Alternatively, coherence effects can be accounted for by building a *dipole* or an *antenna* parton shower, in which the color dipoles radiate coherently [35].

3.1.3 Jet reconstruction algorithms

In practice, experiments cannot exactly reconstruct a parton shower's splitting history from the final state hadron distribution. The hadrons do not come with labels identifying whether or not they come from the same branching history as other hadrons. And, as a stochastic process, all jets will not necessarily be the same. However, the pattern of QCD radiation results in jets with certain well-defined characteristics. Based on this, one can build jet reconstruction algorithms that take a distribution of hadrons and cluster them into jets according to certain criteria. The ensemble of criteria for the clustering of hadrons into a jet is known as the jet definition or jet algorithm, which depends on a number of parameters. Once the parameters or the criteria are changed, the jet definition is changed and the final distribution of jets obtained in a given event may look different. Therefore, a jet should not be confused with the parton shower that produced it. The parton shower is a fundamentally virtual object resulting from the emission of QCD Brehmsstrahlung radiation, whereas a jet is a user-defined object that is built *from* the hadrons that are obtained after the parton shower has ended. This is a great demonstration of the power of MC simulation: the same parton shower definition can be applied to the data from a given collision and to the pseudo-data from an event generator, allowing for direct tests of the underly-

ing physics used to build the parton shower algorithm. Overall, there are two classes of jet algorithms [40]: cone algorithms, based mostly on the geometric characteristics of the particle distributions, and sequential algorithms, which iteratively cluster the hadrons into jets. The latter are the most commonly used ones given that the cone algorithms have been shown to be prone to issues regarding infrared and collinear (IRC) safety. That is, they tend to be more sensitive to the emission of extra soft or collinear particles, unlike an IRC safe algorithm, which guarantees that results obtained at parton level (using perturbation theory) will not dramatically change after hadronization.

One of the most widespread classes of jet algorithms is the generalized $k_{\perp}$ algorithms [40]. They are sequential algorithms defined by a parameter p and a radius(-like) quantity R . With these parameters, the algorithm calculates the following distances between each pair of particles with momenta p_i and p_j :

$$\begin{aligned} d_{ij} &= \min(p_{\perp,i}^{2p}, p_{\perp,j}^{2p}) \frac{\Delta R_{ij}^2}{R^2}, \quad \Delta R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2 \\ d_{iB} &= p_{\perp,i}^{2p}, \\ d_{jB} &= p_{\perp,j}^{2p}, \end{aligned} \tag{3.8}$$

where $y_{i/j}$ is the particle's rapidity and $d_{(i/j)B}$ is the distance between the particle and the beam. The algorithm then calculates these distances for all pairs (i, j) of particles in the event. If d_{ij} is the smallest of the above distances for a given pair, then these two particles are clustered into a single pseudo-particle and the algorithm continues with the updated list of particles. If, at any step, the shortest of the distances in equation (3.8) is one of the $d_{(i/j)B}$, then this (pseudo-)particle is considered a jet and is removed from the list of particles for the next iteration. The algorithm ends once the list of particles is empty.

A few examples of generalized $k_{\perp}$ algorithms are: the **$\mathbf{k}_{\perp}$ algorithm** [42] obtained by setting $p = 1$ such that $d_{ij} = \min(p_{\perp,i}^2, p_{\perp,j}^2)(\Delta R_{ij}^2/R^2)$. Therefore, this algorithm starts by clustering low $p_{\perp}$ particles with each other and gradually builds up to obtain high- $p_{\perp}$ jets. Another possibility is to set $p = 0$, in which case $d_{ij} = (\Delta R_{ij}^2/R^2)$. This is the **Cambridge-Aachen algorithm** [43], and it tends to cluster particles closer in angle first and reaches out to build the jets. Now, recalling the discussion from the previous sections, notice that clustering particles from small to large angles or transverse momenta is, in a way, the inverse process of what the parton shower tends to do given the angular ordering property of QCD radiation. On the other hand, these algorithms often result in jets with irregular shapes. This can pose a challenge for subtracting a background of particles as is often necessary in experiments. This background can come from the underlying event or from pile-up from different collisions. However, the problem becomes worse when going to heavy ion collisions, where the background of soft particles from the multiple nucleon-nucleon interactions can be sizable. Therefore, it is often preferred to cluster jets with the **anti- $\mathbf{k}_{\perp}$ algorithm** [44], which is defined by setting $p = -1$ in equation (3.8). This results in a distance $d_{ij} = (1/\min(p_{\perp,i}^2, p_{\perp,j}^2))(\Delta R_{ij}^2/R^2)$. Therefore, the algorithm tends to cluster particles around the hardest hadrons in the event. As a result, the jet

shape tends to be much closer to a regular cone. This algorithm can be very useful in any type of collisions. However, it is particularly interesting for heavy ion collisions for the aforementioned reason, but, also, because, when the jet evolution happens in a dense environment, the jet-medium interactions break the coherence effects. Therefore, in heavy ion collisions, the consecutive splittings in a parton shower are not necessarily angular ordered and, thus, the motivation to reconstruct jets according to angle is not so strong.

Finally, on the topic of heavy ion collisions, and in light of the discussion in section 2.3, another jet algorithm that can be useful is the **tau algorithm** [19]. This is realized by setting $p = 0.5$ in equation (3.8), such that $d_{ij} = \min(p_{\perp,i}, p_{\perp,j})(\Delta R_{ij}^2/R^2)$. Now, recalling the discussion in section 3.1.1, it can be shown that, for the tau algorithm [45]:

$$d_{ij} \approx p_{\perp,i} \theta^2 \sim \frac{1}{\tau_f}, \quad (3.9)$$

where τ_f is the formation time of the parton with momentum $p_{\perp,i}$, i.e., the time it takes to become an independent source of radiation. Therefore, the iterative steps of clustering particles according to the tau algorithm are (approximately) ordered in time. As a result, this algorithm can be used to study the temporal structure of jets. This was the object of study in paper III in this thesis, in which we explored how the formation time of jets²² can be used as a probe for decoherence effects in collisions of small systems, where the medium might not be dense enough to completely kill off the angular ordering of QCD radiation pattern.

3.2 Monte Carlo for heavy ion collisions

So far in this section, the discussion has been centered around MC event generators with a focus on the parton shower phase of the simulation. Notice that, from the beginning, a central assumption in the modelling of proton-proton interactions is that a given parton can be “picked-out” of the hadron and interact with another isolated parton in the other incoming hadron without being affected by the remnants of the hadrons. In other words, the outgoing partons from a given hard scattering do not rescatter on any other particles. Under this assumption, the energy scales completely factorize and the picture illustrated in Fig. 8 holds. Now, in the case of heavy ion collisions, there may be hundreds of nucleons inside each of the nuclei in the collision. In the worse case scenarios, this could mean thousands of binary proton-proton collisions at each given heavy ion event. Of course the ions are extended objects, nonetheless, when they are accelerated to almost the speed of light, the Lorentz contraction factor can be quite large and, therefore, these binary collisions take place in an extremely dense environment. Therefore, if there happens to be a hard scattering among one of the possibly thousands of proton-proton collisions, it is rather unlikely that the outgoing partons will not be subjected to rescattering. In the absence of a clear obvious choice, a plethora of different models have been built for heavy ions. Many of them build up from the tools described in the beginning of this section

²²I.e., the formation time of the first splitting in the jet history.

and add rescattering effects in different ways, e.g., the ANGANTYR [46] or the JEWEL models [47]. Alternatively, one can take a different route and assume that a thermalized ensemble of partons behaving as a hydrodynamic fluid is quickly formed [48]. The two approaches can also be combined, for example, as in [49].

This is, however, very far from exhausting the wide variety of heavy ion models available and a comprehensive discussion of them is out of the scope of this text. Nonetheless, one common step to almost all the existing heavy ion simulation tools is the Glauber model. This is crucial in setting up the initial conditions for the rest of the evolution and was the object of study of paper II in this thesis. Therefore, let us delve into it in some more detail in the next subsection.

3.3 Glauber models

In section 2, a brief description was given of how Glauber models can be used to compute the thickness of the overlap region (equation (2.2)) between two nuclei. However, the thickness function, as defined in equation (2.2), averages out the granularity of the nuclei. It can still be used to estimate the averaged energy distribution at the initial stages of heavy ion collision events to serve as input, for example, to hydrodynamic simulations. Nonetheless, this formalism is not sensitive to fluctuations that may arise from, for example, the variations in nucleon distributions inside the nuclei. As an alternative, one can make use of the Monte Carlo formulation of the Glauber formalism. These models, known as Monte Carlo Glauber models (MCGs) [50–52] can be used to construct initial conditions, event-by-event, according to the correct probabilities. In general, for a given event, an MCG model does the following:

1. Samples nucleon positions from well known matter distribution functions to build nuclei configurations;
2. Select an impact parameter between the two nuclei, which then fixes the impact parameter between any pair of nucleons;
3. Uses the impact parameter dependent nucleon-nucleon cross sections, $d\sigma_{NN}/d^2b$, to determine the probability for interaction between any two nucleons;
4. Outputs a list of binary collisions with the corresponding participating nucleons and their positions.

Notice that the nucleon-nucleon cross-sections differential in the impact parameter are bound by one [53], which justifies point 3 in the list above. Moreover, their impact-parameter dependence cannot be measured (since no experiment can have direct access to that quantity) and also cannot be computed from first principles (due to involving soft processes that are not calculable in perturbation theory). This means that they must be modelled and fit to the experimentally measured integrated cross-section.

The results of the Glauber model can be fed as initial conditions to different algorithms for heavy ion collision simulations, for example, it can be used to estimate the initial deposition of entropy for hydrodynamic simulations. On the other hand, since the multiplicity can be shown to scale with the number of participating nucleons, it can be used in experiments to relate the measured multiplicity of charge particles to a centrality class²³. It has been shown that the multiplicity distribution across several events is actually rather sensitive to fluctuations [53], especially the high multiplicity tails of such distributions. Paper II of this thesis actually focused precisely on the role of fluctuations in Glauber models by implementing a more realistic impact parameter dependence of the nucleon-nucleon cross sections. The case study of the paper was proton-ion collision. The motivation for that was the fact that, as mentioned in section 2.3, in high multiplicity pA collisions, medium effects have actually been observed. Therefore, in the study of small systems, it is crucial to be able to reproduce these high multiplicity events. Paper II also explored how fluctuations contribute to the anisotropy of the initial conditions in these cases, since, unlike in heavy ion collisions, the impact parameter does not automatically relate to an anisotropic overlapping region.

As for the other papers in this thesis, they also focused on the puzzle of small systems with the use of Monte Carlo models. However, the main focus was on the modification of jets.

3.4 Jet modifications with JEWEL

There is a plethora of models that can contribute to the understanding of jet quenching in heavy ion collisions [54]. In this thesis, one of the main tools used was the JEWEL MC model for jet energy loss [47]. It builds on the PYTHIA 6 [41] event generator but with its own virtuality ordered final state parton shower. It has the great advantage of treating recoils from the splittings locally, which is quite important when the evolution is happening in an expanding medium and the shower must mix momentum and position spaces²⁴. With that, the partons in the shower are allowed to scatter off medium particles in processes described by pQCD t-channel elastic scattering matrix elements, which are regularized by the Debye mass parameter, proportional to the temperature of the medium. It can also account for inelastic scatterings by resetting the parton shower at a higher scale when a parton undergoes a medium scattering at a scale higher than that of the shower. JEWEL has a monopole parton shower and, thus, must account for coherence effects by hand. Angular ordering is taken care of by rejecting splittings that would break it. The version used in this thesis can actually take care of angular ordering in a dynamic manner, such that, if there is a medium scattering between two splitting, angular ordering is not imposed. JEWEL can also account for the LPM effect, which allows for sequential scatterings to act coherently if they happen within the formation time of the following splitting. This new version of JEWEL²⁵ also counts with a mechanism that can take care of coherent emissions in the case

²³Since the impact parameter cannot be measured, the events can be classified in centrality classes based on their multiplicities ranging from most central (0%) to most peripheral (100%).

²⁴Note that, as described in the previous sections, the parton showers are completely built in momentum space. This allows for a more straightforward treatment of recoils, since going back in the shower's ordering variable does not necessarily mean going back in time and, thus, breaking causality.

²⁵The code for this version will be made available at jewel.hepforge.org.

when this emission cannot actually resolve the individual partons in the splitting. All of these new features may not necessarily have strong consequences for heavy ion collisions, but, as shown in papers III and IV in this thesis, they can allow for the study of observable coherence effects in small systems.

3.5 Small systems again

As discussed in section 2.3, several medium signatures have been observed in collisions of small systems. This has motivated attempts to use hydrodynamic models in small systems [55], although such attempts seem to carry serious problems [56–58]. Therefore, the question arises of how to treat such systems.

The JEWEL model described above was originally formulated for the study of heavy ion collisions. However, it is very flexible about its medium definition. One can couple JEWEL to different medium models, even hydrodynamic ones [59]. This makes it a powerful tool in the study of jet quenching (or absence thereof) in small systems, where the medium is not very well understood.

In this thesis, papers I, III and IV make use of this flexibility of JEWEL in order to study small systems. From the minimal brick-like medium in paper I to the sophisticated hydrodynamic model used in the study of coherence in paper IV, we have explored qualitatively and quantitatively the sensitivity of different observables to coherence effects and medium interactions in small systems.

4 Conclusions and Outlook

*Tem que chorar no começo pra sorrir no fim.**

— Marta

Heavy ion collisions provide a rich playing ground for the study of QCD phenomenology. The high energies and densities probed in these collisions allow for the onset of asymptotic freedom and the formation of a medium composed of quarks and gluons. However, the rapid re-establishment of confinement poses a challenge for the study of this medium. In this context, Monte Carlo event generators emerge as perfect tools to facilitate tests of theoretical predictions based on perturbative methods against experimental observations of the confined final states of these collisions. Although the medium cannot be directly observed, its formation and evolution leave strong signatures in the final state hadron distributions. As a result, the existence of this medium was not only confirmed, but it was identified as a liquid-like fluid of quarks and gluons. Nonetheless, many of these signatures were also observed in collisions of small systems where no medium was believed to be formed. However, no jet quenching has been observed even when signs of collectivity were present. This

*Own translation: “Cry at the beginning so you can smile at the end.”

apparently contradictory scenario is commonly referred to as the puzzle of small systems. Reconciling the absence of energy loss with the presence of medium signatures in small systems remains an open question in the field. It challenges not only the interpretation of these signatures in heavy ion collisions but also the assumptions of the well-established proton-proton collision models in which no final state rescatterings are present. All the works in this thesis are related to this open question.

In paper I, it was shown, in a quantitative study, that the sensitivity of high- $p_{\perp}$ v_2 and jet R_{AA} to medium interactions is actually remarkably similar. However, this study also showed that the dynamics of jet energy loss can lead to different R_{AA} signatures. In other words, when the same amount of energy loss is confined in the early stages of the parton shower, it can lead to a different result compared to the same energy loss spread out in a larger region. These results, as well as other evidence already present in the literature, show that a more detailed study of the jet energy loss process is required. This motivates the development of a new observable that can probe the temporal structure of jets, for example, the formation time. Paper III explored this new observable and showed that it is sensitive to the breaking of color coherence due to medium interactions, even in the case when such scatterings are so soft that no energy loss is actually observed. With this evidence that color coherence may actually be probed in small systems, paper IV then expands on it. In that case, it was shown that color coherence can affect how jets lose energy inside the medium. On the other hand, paper II tackles the puzzle from a different perspective and shows that a proper treatment of fluctuations in Glauber models may actually lead to large anisotropies in small systems.

These results open several avenues for further studies. Paper I touched on the sensitivity of R_{AA} and v_2 to the dynamics of energy loss. This can be further expanded with the help of a toy model to understand how the scattering angle and energy transfer affect these two observables separately. As for paper III, we will continue exploring the formation time as a probe for medium formation in small systems, but with a focus on how it is affected when energy loss is significant. The Glauber model conceived in paper II can also be expanded to for ion-ion collisions and put to test in a more complete scenario.

Nevertheless, all the results presented in papers I-IV strongly indicate that the absence of jet quenching in small systems is not necessarily contradictory with the presence of a high- $p_{\perp}$ v_2 , although they are both caused by energy loss. In fact, this apparent contradiction tends to vanish with the proper treatment of color coherence and/or of cross-section fluctuations. In other words, we must use the adequate observables for the appropriate systems.

In all, the heavy ion community has only just begun to bridge the gap between the very dilute and very dense systems. The work that lies ahead depends on the development of the proper observables that allow us to understand the space-time evolution of the medium. Hard probes continue being a powerful tool in this endeavor and a detailed understanding of the internal structure and evolution of jets will pave the way towards a complete and coherent picture of heavy ion phenomenology across different system sizes.

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Overview of publications

This thesis is based on the following scientific papers:

Paper I

How many interactions does it take to modify a jet?

Chiara Le Roux, José Guilherme Milhano, Korinna Zapp

Eur. Phys. J. C 85, 1065 (2025)

e-print: arXiv:2412.14983 [hep-ph]

In this publication, we aim to reconcile the contrasting observation of a high- $p_{\perp}$ v_2 with the absence of jet R_{AA} suppression in small systems. For that, we found a common scaling quantity for both the observables which is completely independent of the medium model, thus suitable for the case of small systems, where little is known about the evolution of the existing medium. We study the braking of this scaling and contribute to understanding the dynamics of jet energy loss in small systems.

I have done the main work in this paper. This included writing the code for the analysis and, with the support of my supervisor, the code for the medium model used in this work. I produced the results in figures 1, 2 and 4 and table 1. I have contributed to the interpretation of the results and ideas such as trying other scaling variables for example. Furthermore, I have written the introduction and results and given contribution to the text in the other sections as well.

Paper II

How cross section fluctuations affect multiplicity and geometry in pA collisions

Chiara Le Roux

Submitted to Eur. Phys. J. C

e-print: arXiv:2507.21843 [hep-ph]

In this paper, a Glauber model was built from the cross-sections calculated within the KMR/SHRiMPS model. Besides being a well motivated calculation of soft QCD observables, this model has the advantage that it naturally provides a non-trivial impact parameter dependence to the cross-sections. This introduces an additional source of fluctuations which, as was shown in the paper, impacts not only the number of binary collisions, but also their spacial distribution.

I have implemented the code and produced all the results presented in this paper as well as written all the text, to which my supervisor gave feedback.

Paper III

Jet quenching without energy loss

Liliana Apolinário, Chiara Le Roux, Korinna Zapp

Submitted to Phys. Lett. B

e-print: arXiv:2510.11914 [hep-ph]

In this publication, we explored the possibility of using the formation time of jets as a probe for color decoherence. We show that the theory actually predicts different distributions for the formation times of jets when color coherence takes place and when some mechanism, e.g., medium interactions, break the coherence of color particles. Additionally, we investigate the possibility of reconstructing this signal after the hadrons are reclustered into jets with a commonly used jet algorithm and unclustered with the formation time algorithm. It was shown that, although the signal is less strong after reconstruction it is still there and could, therefore, be used to look for decoherence of color particles in experimental situations.

I have produced the main work for this paper. That included writing the analysis code and producing all the figures in the paper. I have also substantially contributed to the interpretation of the results and written the results section and partially written the “model” section of this paper as well as helped revise the complete text.

Paper IV

Colour coherence in small collision systems

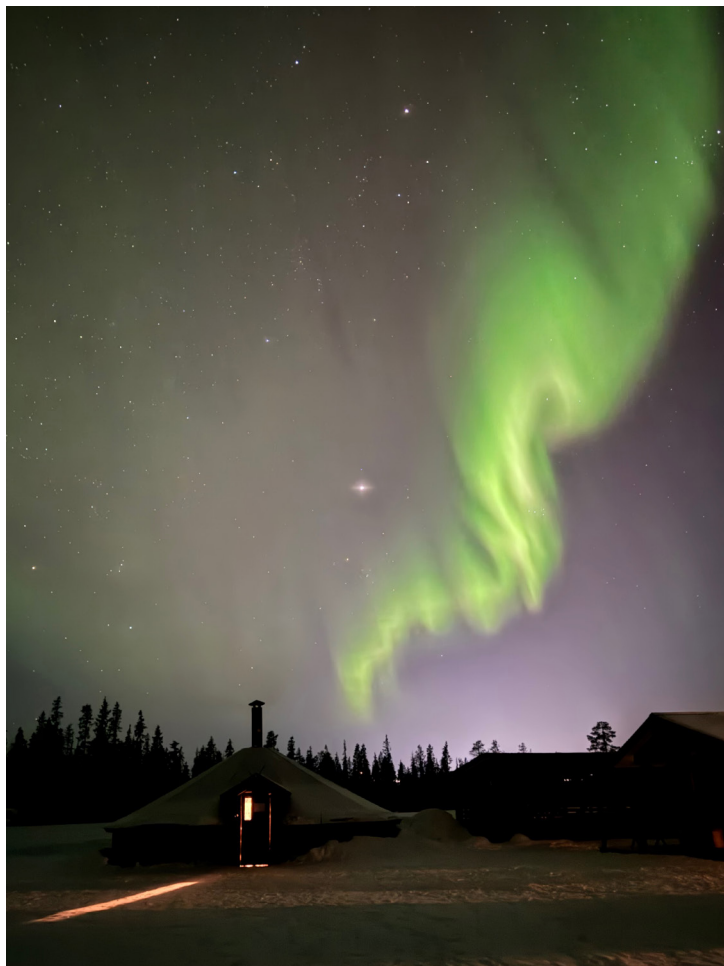
Isobel Kolbé, Chiara Le Roux, Korinna Zapp

To be submitted

e-print: arXiv:2510.17570 [hep-ph]

In this paper we investigated the effect of colour coherence in collisions of small systems. We studied both jet and hadron R_{AA} as well as v_2 . It was shown that coherence contributes for an increase in R_{AA} but do not affect v_2 as much. We have also studied the effect of the system shape in R_{AA} using a hydrodynamic medium model.

For this paper, I have contributed with the coding of the hadron R_{AA} analysis as well as to the discussions of the results and how to move forward. I have contributed substantially to the writing of the paper especially of sections 1, 2 and 3.



*“Se a educação sozinha não transforma a sociedade,
sem ela tampouco a sociedade muda.”*

“If education alone cannot transform society, without it society cannot change either.”

— Paulo Freire, Pedagogia da Indignação