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Computational tools for perturbative calculations in renormalization of Hamiltonian

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Resumen

El procedimiento del grupo de renormalización para partículas efectivas juega un papel fundamental en la comprensión de fenómenos físicos a distintas escalas, construyendo teorías efectivas que capturan las interacciones más relevantes dentro de un rango de energía determinado. Se construyen Hamiltonianos efectivos a partir de un Hamiltoniano inicial y una transformación unitaria dependiente de la escala.

Para resolver las ecuaciones planteadas, se requiere de un tratamiento perturbativo, siendo útil e intuitivo representar los distintos términos de la teoría como diagramas que describen el tipo de interacción, de forma análoga a los diagramas de Feynman. Como el número de diagramas aumenta exponencialmente con el orden de la perturbación, el proceso de cálculo es tedioso y propenso a errores.

El objetivo de este trabajo es desarrollar un programa [1] que automatice el proceso de obtención de diagramas asociados a un término de interacción y orden determinado, partiendo de unos diagramas base, o canónicos de la teoría elegida.

El programa es capaz de descartar los diagramas que no contribuyen a la interacción de interés, detectar loops y añadir contraterminos a los diagramas para cancelar divergencias. Analizando los diagramas obtenidos de ordenes inferiores, y comparando con resultados conocidos, se ha comprobado la validez del programa. Esto permite obtener los diagramas de ordenes superiores, y estudiar el aspecto del comportamiento de la teoría a dichos ordenes, donde emergen características distintivas de las teorías gauge no abelianas.

Abstract

The renormalization group procedure for effective particles plays a fundamental role in understanding physical phenomena at different scales, constructing effective theories that capture the most relevant interactions within a certain energy range. Effective Hamiltonians are constructed from an initial Hamiltonian and a scale-dependent unitary transformation.

Often, a perturbative treatment is required to solve the renormalization-group equations, and it's useful and convenient representing the different terms of the theory as diagrams that describe the process, in analogy with Feynman diagrams. However, the number of diagrams increases exponentially with the order of the perturbation, making the calculation process tedious and error-prone.

The aim of this work is to develop a program [1] that automates the process of obtaining the diagrams associated with a given interaction term, and at a given order, starting from the set of base diagrams, given by the canonical Hamiltonian of the theory.

The program is able to discard the diagrams that do not contribute to the desired interaction, detect loops and add counterterms to the divergent contributions. By analyzing the diagrams obtained from lower orders, and comparing with known results, the correctness of the program has been verified. This allows to obtain the diagrams of higher orders, and study the behavior of the theory at those orders, where distinct features of non-Abelian gauge theories emerge.

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1 Introduction

When building a theory that describes the particles and their interactions, it's imperative that the theory be compatible with the two pillars of modern physics: special relativity and quantum mechanics. Special relativity is a theory that describes the behavior of particles at high energies, and quantum mechanics is a theory that describes the behavior of particles at atomic and subatomic scales. Combining these two frameworks leads to quantum field theory (QFT), a formalism in which particles are interpreted as excitations of underlying fields.

Quantum Chromodynamics (QCD) is the quantum field theory that describes the strong interaction in terms of quarks and gluons. This theory has proven to be extremely difficult to use in practice. Many alternative strategies have arisen with the purpose of addressing different aspects of the theory while neglecting those less relevant to specific problems.

An important aspect of any theoretical approach to QCD is that it should be able to describe phenomena occurring at different energy scales. At low energies (long distances), experiments reveal only bound states, hadrons, whose internal structure is effectively smoothed out. At high energies (short distances), one can probe inside hadrons, where quarks and gluons behave almost as free particles, a phenomenon known as asymptotic freedom. The theory must interpolate between these regimes.

In the context of theoretical physics, the renormalization group procedure for effective particle (RGPEP) is a powerful tool formulated in Hamiltonian dynamics to study the behavior of physical systems across different energy scales [2]. In the case of quantum field theories, the renormalization group procedure introduces a scale parameter, which moderates the "resolution" of the system, allowing one to focus on specific energy scales, from the smallest details (the short distance behavior) to the largest ones (the large-scale behavior).

The RGPEP yields an effective Hamiltonian, that describes the system at a given scale. This effective Hamiltonian is the solution to a differential equation, the RGPEP equation, which governs the evolution of the effective Hamiltonian with respect to the scale parameter. In general, obtaining the exact solution to the RGPEP equation is a non-trivial task, and a perturbative expansion of the effective Hamiltonian is used to obtain the solution. [3]

Every interaction term in the Hamiltonian can be identified with a diagram, which, in turn, results as a product of diagrams of lower order. These diagrams are usually drawn by hand, but the abundance of diagrams grows exponentially with the increasing perturbative order, making the process tedious and error-prone. The goal of this thesis is to develop a tool that automates the process of obtaining the diagrams associated with a certain interaction for a given order.

The program is designed from the ground up, using some basic python libraries, and to my knowledge, it's the first for this specific application. Similar programs exist for covariant Feynman diagrams [4, 5], but they are not suitable for the RGPEP.

This thesis is organized as follows. Section 2 describes the theoretical background needed to understand the renormalization group procedure for effective particles in the context of Hamiltonian dynamics. Section 2.3 describes the example studied in this thesis, gluon interactions. Choosing this example we simplify the theory by keeping only one type of particle, while some peculiarities of QCD are explicitly considered. Section 3 describes how diagrams are defined in the code, and Section 4 describes the steps taken to obtain diagrams of arbitrary order, as product of elementary ones. Finally, Section 5 presents the conclusions, possible future work and further improvement to the code, which is available online in the repository [1].

2 Theoretical background

To understand the basis of the RGPEP, we need to describe the different concepts involved in the framework, as well as the theories that the process is applied to.

2.1 Fock space

In quantum field theory, the number of particles is not conserved and processes such as particle creation and annihilation occur. The formal description of such features operates on the Fock space [6]. The Fock space is a sum of different Hilbert spaces, each one corresponding to a different number of particles, thus allowing the description of quantum systems with a variable number of particles.

The Fock space is defined as the direct sum of tensor products of the single particle Hilbert space \mathbb{H} ,

$$\mathbb{F} = \bigoplus_{n=0}^{\infty} \mathbb{H}^{\otimes n} = \mathbb{C} \oplus \mathbb{H} \oplus (\mathbb{H} \otimes \mathbb{H}) \oplus (\mathbb{H} \otimes \mathbb{H} \otimes \mathbb{H}) \oplus \cdots, \quad (2.1)$$

where \mathbb{C} is the complex scalar, corresponding to the states with no particles, and each terms $\mathbb{H}^{\otimes n}$ represent the Hilbert space for n -particle states.

This way a general state in the Fock space can be expressed as,

$$|\Psi\rangle = |\Psi_0\rangle \oplus |\Psi_1\rangle \oplus |\Psi_2\rangle \oplus \cdots = c|0\rangle + \sum_{i=1} c_i |\psi_i\rangle + \sum_{i,j=1} c_{ij} |\psi_i \psi_j\rangle + \cdots, \quad (2.2)$$

where $|\Psi_0\rangle$ is the vacuum state, $|\Psi_1\rangle$ is the one particle state, $|\Psi_2\rangle$ is the two particle state, and so on. The coefficients c_i are the amplitudes of the states, in general, complex numbers.

Fock space provides a natural framework for quantum field theories, where, physical states are expressed as superposition of all allowable multiparticle configurations consistent quantum numbers. For instance, a quarkonium state (a bound state of quark and antiquark) in QCD is given by:

$$|\Psi\rangle = c_1 |q\bar{q}\rangle + c_2 |q\bar{q}g\rangle + c_3 |q\bar{q}gg\rangle + \cdots, \quad (2.3)$$

2.2 Hamiltonian dynamics

In quantum field theory, two equivalent formulations of the dynamics can be used, the Lagrangian and the Hamiltonian formulations. Although one often starts with a Lagrangian formulation and then switches to a Hamiltonian via a Legendre transform, here we adopt the Hamiltonian (canonical) formalism because RGPEP works on the operator space, and thus it is implemented in Hamiltonian dynamics. These operators act on the Fock space.

2.2.1 Noether's theorem

A Hamiltonian can be derived from the Lagrangian of the theory by the means of Noether's theorem [7, 8]. It states that every continuous symmetry of the Lagrangian of a physical system corresponds to a conserved quantity. In the context of quantum field theory, this theorem is fundamental as it relates symmetries of the Lagrangian to conservation laws, which are crucial for understanding the dynamics of the system.

Considering a general continuous transformation of the fields $\phi_a(x) \rightarrow \tilde{\phi}_a(x)$ ¹, which in the infinitesimal form can be expressed as,

$$\phi_a(x) \rightarrow \tilde{\phi}_a(x) = \phi_a(x) + \delta\phi_a(x) = \phi_a(x) + \epsilon Q_a(x), \quad (2.4)$$

where ϵ is an infinitesimal parameter, and $Q_a(x)$ is some deformation of the field. This transformation is a symmetry if it leaves the equations of motion invariant, which means that the Lagrangian density $\mathcal{L}(\phi_a, \partial_\mu \phi_a)$ remains unchanged under such transformation, up to a four-divergence of some current J^μ ,

$$\mathcal{L}(\tilde{\phi}_a, \partial_\mu \tilde{\phi}_a) = \mathcal{L}(\phi_a, \partial_\mu \phi_a) + \epsilon \partial_\mu J^\mu. \quad (2.5)$$

The conserved current j^μ is defined as the Noether current associated with the symmetry transformation, which is given by,

$$j^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi_a)} Q_a - J^\mu, \quad \partial_\mu j^\mu = 0, \quad (2.6)$$

where Einstein summation is assumed.²

Applying Noether's theorem, the conserved charge Q associated with the symmetry is defined as the integral of the time component of the current over all space:

$$Q = \int d^3x j^0(x). \quad (2.7)$$

Applying Noether's theorem to translations, in infinitesimal form,

¹where x indicate a 4-vector in Minkowski space, with x^μ its components, and $\partial_\mu = \frac{\partial}{\partial x^\mu}$

²The Einstein summation convention is a notational convention in which repeated indices in a mathematical expression imply contraction over those indices, by the use of the Minkowski metric $g^{\mu\nu}$. For example, $A^\mu B_\mu = g_{\mu\nu} A^\mu B^\nu = A^0 B^0 - \sum_i A^i B^i$

$$x^\mu \rightarrow \tilde{x}^\mu = x^\mu + \epsilon \mathcal{A}^\mu, \quad (2.8)$$

where \mathcal{A}^μ is a vector that represents the infinitesimal translation, the transformation of the fields is given by,

$$\phi_a(x) \rightarrow \tilde{\phi}_a(\tilde{x}) = \phi_a(x) + \epsilon \mathcal{A}^\mu \partial_\mu \phi_a(x). \quad (2.9)$$

The Lagrangian density transforms as,

$$\mathcal{L} \rightarrow \mathcal{L} + \epsilon \mathcal{A}^\nu \partial_\nu (\delta_\nu^\mu \mathcal{L}), \quad (2.10)$$

Comparing with equation (2.5), four different conserved currents can be identified,

$$T^\mu_\nu = \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi_a)} \partial_\nu \phi_a - \delta^\mu_\nu \mathcal{L}. \quad (2.11)$$

This is the energy-momentum tensor of the field. The conserved charge associated with the time translation symmetry is the Hamiltonian H ,

$$H = \int d^3x T^{00}(x) = \int d^3x \mathcal{H}, \quad (2.12)$$

and the conserved charges associated with the spatial translations,

$$P^i = \int d^3x T^{0i}(x), \quad (2.13)$$

which it is interpreted as the physical momentum operator.

One can proceed analogously to obtain the angular momentum and boost operators. All together form the ten generators of the Poincaré group.

2.2.2 Canonical Hamiltonian

An equivalent derivation of the Hamiltonian, is done by defining the canonical conjugate momenta [8],

$$\pi_a(x) = \frac{\partial \mathcal{L}}{\partial (\partial_0 \phi_a(x))}. \quad (2.14)$$

The associate Hamiltonian density, which is equivalent to Eq.(2.12), can be written as,

$$\mathcal{H} = \pi_a(x) \partial_0 \phi_a(x) - \mathcal{L}(\phi_a(x), \partial_\mu \phi_a(x)), \quad (2.15)$$

and the momentum,

$$P^i = \int d^3x T^{0i}(x) = \int d^3x \pi_a(x) \partial^i \phi_a(x). \quad (2.16)$$

In quantum mechanics, or quantum field theory, the canonical coordinate $\phi_a(x)$ and the momentum conjugate $\pi_a(x)$ are promoted to operators acting on a Hilbert space. Quantization is achieved by imposing equal-time canonical commutation relations [9],

$$[\phi_a(x), \pi_b(y)] = i\delta_{ab}\delta^3(x-y), \quad [\phi_a(x), \phi_b(y)] = 0, \quad [\pi_a(x), \pi_b(y)] = 0. \quad (2.17)$$

The field operators are expanded in terms of creation, a_i and annihilation a_i^\dagger operators, that act on the Fock space, creating and annihilating the mode i of the field. Mathematically, the creation and annihilation operators are the Fourier components of the field.

Any state component in the Fock space can be expressed as the action of a series of creation operators on the vacuum state, $|0\rangle$,

$$|\Psi_n\rangle = \sum_{i_1, i_2, \dots, i_n} \frac{c_{i_1 i_2 \dots i_n}}{\sqrt{n!}} a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger |0\rangle, \quad (2.18)$$

making the full state,

$$|\Psi\rangle = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \sum_{i_1, i_2, \dots, i_n} c_{i_1 i_2 \dots i_n} a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger |0\rangle. \quad (2.19)$$

The creation and annihilation operators satisfy some commutation or anticommutation relations, depending on the nature of the particles, bosons or fermions, respectively, according to (2.17).

For bosons, the creation and annihilation operators satisfy the following commutation relations,

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = 0, \quad [a_i^\dagger, a_j^\dagger] = 0. \quad (2.20)$$

For fermions, the creation and annihilation operators satisfy the following anticommutation relations,

$$\{q_i, q_j^\dagger\} = \delta_{ij}, \quad \{q_i, q_j\} = 0, \quad \{q_i^\dagger, q_j^\dagger\} = 0. \quad (2.21)$$

This way, the creation and annihilation operators are the fundamental objects acting on the Fock space, and the Hamiltonian and the fields are expressed in terms of these operators.

When a combination of creation and annihilation operators is considered, normal-ordering is used when defining operators that contain both creation and annihilation operators. The normal-ordering is defined as the process of rearranging the creation and annihilation operators in such a way that all the creation operators are to the left of all the annihilation operators.

2.2.3 Front Form of Hamiltonian Dynamics

The quantization of relativistic systems is most commonly performed in the instant form (IF) of dynamics, where the ordinary time coordinate $x^0 = t$ serves as the evolution parameter, and spatial coordinates \vec{x} define the hypersurface of equal time. The quantization surface (where the initial conditions are defined) is given by $x^0 = 0$. However, alternative forms of dynamics are possible and were classified by Dirac in 1949 [10].

One such alternative is the front form (FF) of dynamics, also known as light-front quantization. It is defined by choosing a new set of coordinates where the evolution parameter is,

$$x^+ = \frac{1}{\sqrt{2}}(x^0 + x^3), \quad (2.22)$$

and the remaining coordinates are,

$$x^- = \frac{1}{\sqrt{2}}(x^0 - x^3), \quad x^\perp = (x^1, x^2). \quad (2.23)$$

In this framework, quantization is performed on surfaces of constant x^+ , typically $x^+ = 0$, treating it as the "light-front time", while x^-, x^\perp play the role of spatial coordinates. The corresponding momenta are defined as,

$$p^+ = \frac{1}{\sqrt{2}}(p^0 + p^3), \quad p^- = \frac{1}{\sqrt{2}}(p^0 - p^3), \quad p^\perp = (p^1, p^2). \quad (2.24)$$

The light-front Hamiltonian P^- is derived from the conserved charge related to the component x^+ , following a similar procedure as before. It governs the evolution in x^+ , analogous to the role of $H = P^0$ in instant-form quantization.

A key feature of FF quantization is the positivity condition $p^+ > 0$ for all physical particles.³ This kinematic constraint ensures that particle creation from the vacuum, which has total $P^+ = 0$, is forbidden due to momentum conservation. As a result, the vacuum in FF is trivial or "empty" [12]: it contains no virtual particles and cannot mix with multi-particle states.

This property simplifies drastically the structure of the theory, where a clean separation between the vacuum and the particle spectrum is advantageous. Hence, FF quantization avoids the complexities associated with vacuum fluctuations that are typical in instant-form dynamics.

³Although gluons are supposed to be massless and therefore this condition does not hold for them, in practice, it is assumed here to have infinitesimally small mass (which is taken to zero at the end of the calculation) [11].

2.3 Case study: Gluons self-interactions

2.3.1 Quantum Chromodynamics (QCD)

QCD is the quantum field theory that describes the interactions of quarks and gluons, the fundamental constituents of hadrons. It is a non-abelian gauge theory based on the $SU(3)$ gauge group [13].

The Lagrangian for QCD is given by,

$$\mathcal{L}_{QCD} = -\frac{1}{4}F^{a,\mu\nu}F_{\mu\nu}^a + \bar{\psi} (i\gamma^\mu D_\mu - m) \psi, \quad (2.25)$$

where $F^{a,\mu\nu}$ is the field strength tensor for the gluon fields,

$$F^{a,\mu\nu} = \partial^\mu A^{a,\nu} - \partial^\nu A^{a,\mu} + gf^{abc}A^{b,\mu}A^{c,\nu}, \quad (2.26)$$

$A^{a,\mu}$ are the gluon fields, ψ is the quark field, m is the quark mass, and D_μ is the covariant derivative defined as,

$$D_\mu = \partial_\mu - igA_\mu^a t^a, \quad (2.27)$$

where t^a are the generators of the $SU(3)$ gauge group, and g is the coupling constant of the strong interaction.

The structure constants f^{abc} encode the non-abelian nature of the theory, and are present explicitly in the commutation relations of the generators of the gauge group,

$$[t^a, t^b] = if^{abc}t^c, \quad (2.28)$$

as well as in the Hamiltonian, in the interacting terms involving the gluon fields.

2.3.2 Canonical Hamiltonian for the gluon fields

For our purposes, we will focus on the gluon fields. The Lagrangian density for the gluon fields is given by the first term of the QCD Lagrangian (2.25),

$$\mathcal{L} = -\frac{1}{2}\text{tr}F^{\mu\nu}F_{\mu\nu}, \quad (2.29)$$

We will be working in the gauge $A^+ = 0$ ⁴, where the Lagrange equations constrain the component A^- to become,

$$A^- = \frac{1}{\partial^+}2\partial^\perp A^\perp - \frac{2}{\partial^{+2}}ig\left[\partial^+ A^\perp, A^\perp\right]. \quad (2.30)$$

In this way, the only degree of freedom left is the transverse component A^\perp ⁵.

As for the associated energy-momentum tensor,

⁴Here $A^+ = 0$ is a convenient choice of gauge on the light front which eliminates unphysical degrees of freedom. The equation above is the result of the Euler-Lagrange constraint for A^- in this gauge, ensuring A^- is not an independent field.

⁵Similar to before, the vectors in FF have components $A^\mu = (A^+, A^-, A^\perp)$, where $A^\perp = (A^1, A^2)$.

$$\mathcal{T}^{\mu\nu} = -F^{a\mu\alpha}\partial^\nu A_\alpha^a + \frac{1}{4}g^{\mu\nu}F^{\alpha\beta}F_{\alpha\beta}. \quad (2.31)$$

The Hamiltonian in FF quantization is obtained from integrating the component \mathcal{T}^{+-} of the energy-momentum tensor, over the hyperplane $x^+ = 0$.

By working in the gauge $A^+ = 0$, the Hamiltonian density can be expressed as the sum of four terms, as denoted in [14]

$$\mathcal{T}^{+-} = \mathcal{H}_{A^2} + \mathcal{H}_{A^3} + \mathcal{H}_{A^4} + \mathcal{H}_{[\partial AA]^2}, \quad (2.32)$$

with each of the terms,

$$\mathcal{H}_{A^2} = -\frac{1}{2}A^{\perp a}(\partial^\perp)^2 A^{\perp a}, \quad (2.33)$$

$$\mathcal{H}_{A^3} = gi\partial_\alpha A_\beta^a [A^\alpha, A^\beta]^a, \quad (2.34)$$

$$\mathcal{H}_{A^4} = -\frac{1}{4}g^2 [A_\alpha, A_\beta]^a [A^\alpha, A^\beta]^a, \quad (2.35)$$

$$\mathcal{H}_{[\partial AA]^2} = -\frac{1}{2}g^2 [i\partial^+ A^\perp, A^\perp]^a \frac{1}{(i\partial^+)^2} [i\partial^+ A^\perp, A^\perp]^a. \quad (2.36)$$

Replacing A^μ with the operator $\hat{A}^\mu(x)$, defined by its Fourier composition on the plane $x^+ = 0$,

$$\hat{A}^\mu(x) = \sum_{\sigma c} \int [k] \left[t^c \epsilon_{k\sigma}^\mu a_{k\sigma c} e^{-ikx} + t^c \epsilon_{k\sigma}^{\mu*} a_{k\sigma c}^\dagger e^{ikx} \right]_{x^+=0}, \quad (2.37)$$

where $[k] = \theta(k^+)dk^+d^2k^\perp/(16\pi^3k^+)$, $\epsilon_{k\sigma}^\mu$ are the polarization vectors, and $a_{k\sigma c}^\dagger$, $a_{k\sigma c}$ are the creation and annihilation operators (also called particle operators), respectively.

Substituting this expression into each term of the Hamiltonian densities, integrating over space coordinates and taking into account the completeness and orthonormality of the polarization vectors, one obtains the following expression for the different terms of the Hamiltonian [3],

$$H_{A^2} = \sum_{\sigma c} \int [k] \frac{k^{\perp 2}}{k^+} a_{k\sigma c}^\dagger a_{k\sigma c}, \quad (2.38)$$

$$H_{A^3} = \sum_{123} \int [123] \not{\epsilon}(p^\dagger - p) g \left[Y_{123} a_1^\dagger a_2^\dagger a_3 + Y_{123}^* a_3^\dagger a_2 a_1 \right], \quad (2.39)$$

$$H_{A^4} = \sum_{1234} \int [1234] \not{\epsilon}(p^\dagger - p) \frac{g^2}{4} \left[\left(\Xi_{A^4 1234} a_1^\dagger a_2^\dagger a_3^\dagger a_4 + h.c. \right) + X_{A^4 1234} a_1^\dagger a_2^\dagger a_3 a_4 \right], \quad (2.40)$$

$$H_{[\partial AA]^2} = \sum_{1234} \int [1234] \not{\epsilon}(p^\dagger - p) g^2 \left[\left(\Xi_{[\partial AA]^2 1234} a_1^\dagger a_2^\dagger a_3^\dagger a_4 + h.c. \right) + X_{[\partial AA]^2 1234} a_1^\dagger a_2^\dagger a_3 a_4 \right]. \quad (2.41)$$

Here the notation $[123]$ indicates the integration over the momenta of the particles 1 to 3, $[123] = [k_1][k_2][k_3]$. The explicit expression for the functions Ξ, Y, X, \dots , can be found in [3], for the purpose of this thesis, we are only interested in the dependence of the functions on the structure constant f^{abc} .

The terms H_{A^2} , H_{A^3} , H_{A^4} and $H_{[\partial AA]^2}$ represent the different interaction terms of the gluon fields: H_{A^2} corresponds to the kinetic term of the gluon fields, H_{A^3} corresponds to the three-gluon vertex and H_{A^4} together with $H_{[\partial AA]^2}$ corresponds to four-gluon vertices.

In the context of light-front QCD, the four-gluon vertices can be treated as a combination of two time ordered three-gluon vertices, or as a special case of instantaneous interaction.

As for the dependence on the coupling constant g , the term H_{A^2} can be seen as an order zero term, since it does not contain the coupling constant g . The term H_{A^3} , Eq.(2.39) is a first-order term, since it contains g to the first power, as well as a single structure constant f^{abc} . The diagram representation of this term is shown in figure 1. These diagrams represent the process of 1 gluon going to 2 gluons (Fig. 1a), and its hermitian conjugate of 2 gluons going to 1 gluon (Fig. 1b).

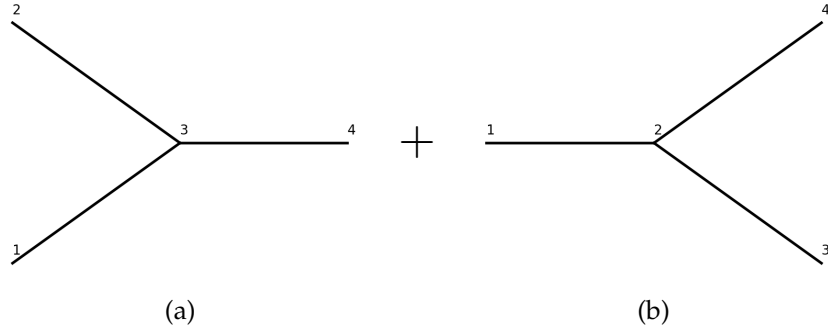


Figure 1: Canonical diagrams that go with g

While the term H_{A^4} and $H_{[\partial AA]^2}$ are second order term, since they contain g^2 to the second power, and two structure constants. The diagrams obtained are shown in figures 2, 3 and 4. Each of these diagrams corresponds to a different term in the Hamiltonian, contributing to different processes.

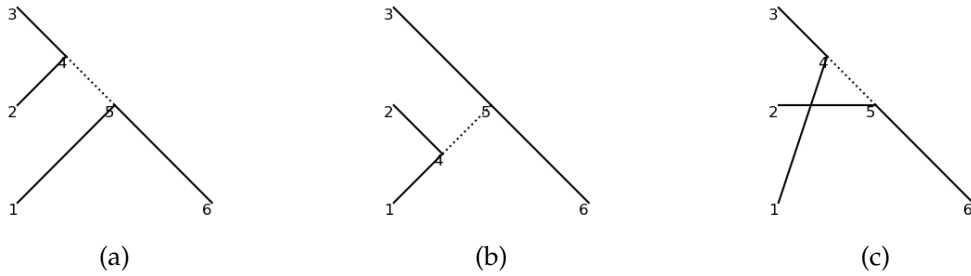


Figure 2: Canonical diagrams that go with g^2 in the term $\Xi_{[\partial AA]^2}$, where one gluon is annihilated, and 3 gluons are created.

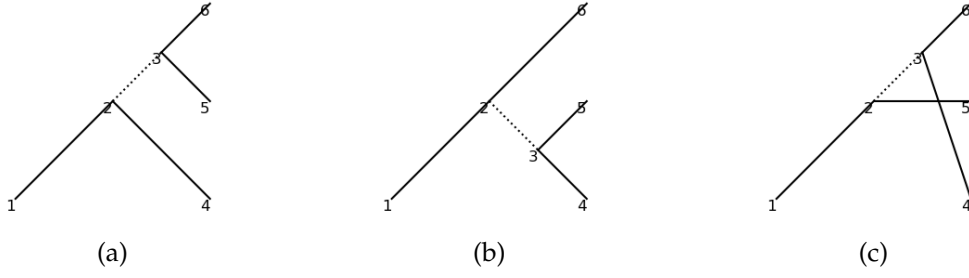


Figure 3: Canonical diagrams of order 2, for the term Hermitian conjugate with coefficient $\Xi_{[\partial AA]^2}^*$, where 3 gluons are annihilated, and 1 gluon is created.

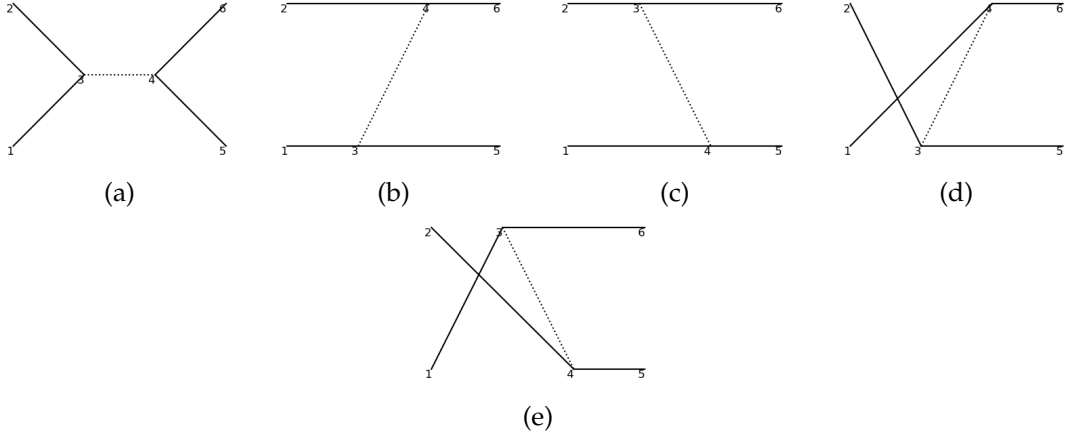


Figure 4: Canonical diagrams of order 2, for the term $X_{[\partial AA]^2}$, where 2 gluons are annihilated, and 2 gluons are created.

2.4 Renormalization group procedure for effective particles (RGPEP)

The RGPEP, is a renormalization group procedure applied within the Hamiltonian formulation of quantum field theory, formulated by S.D.Głazek and K.G.Wilson [2, 15–17]. By considering a series of unitary transformations applied to the canonical or bare Hamiltonian, the RGPEP is able to construct a succession of effective Hamiltonians \mathcal{H}_s , each describing dynamics in terms of effective particles at a resolution scale set by the parameter s . This is associated with the renormalization group scale $\lambda = 1/s$, where λ has dimension of energy, and has the interpretation of the characteristic energy scale of the theory, while s has dimension of length, and has the interpretation of the *size* of effective particles.

Effective particles, are defined by effective-particle operators that differs from the canonical ones by the unitary transformation \mathcal{U}_s ,

$$a_s = \mathcal{U}_s a_0 \mathcal{U}_s^\dagger. \quad (2.42)$$

Due to dimensional and notational reasons, it is convenient to consider the scale parameter $t = s^4$ instead.

Then, for $s = 0$ or, equivalently, $t = 0$, the theory describes point-like or bare particles, those associated to the canonical Hamiltonian $\mathcal{H}_0(a_0)$.

The effective Hamiltonian \mathcal{H}_t , written in terms of the effective particle operator a_s , is related to the regulated canonical Hamiltonian with counter-terms by the condition (section 2.4.1),

$$\mathcal{H}_t(a_t) = \mathcal{H}_0(a_0), \quad (2.43)$$

Using Eq. (2.42) and expressing all operators in terms of the original a_0 , the effective Hamiltonian becomes,

$$\mathcal{H}_t(a_0) = \mathcal{U}_t^\dagger \mathcal{H}_0(a_0) \mathcal{U}_t. \quad (2.44)$$

Differentiating with respect of t , one obtains the RGPEP differential equation,

$$\mathcal{H}'_t(a_0) = \frac{d}{dt} \mathcal{H}_t(a_0) = \left[-\mathcal{U}_t^\dagger \mathcal{U}'_t, \mathcal{H}_t(a_0) \right] \equiv [\mathcal{G}_t(a_0), \mathcal{H}_t(a_0)], \quad (2.45)$$

where \mathcal{G}_t is the generator of the RGPEP transformation.

Considering the generator from Ref. [18],

$$\mathcal{G}_t = [\mathcal{H}_f, \mathcal{H}_{Pt}], \quad (2.46)$$

where \mathcal{H}_f is the free part of \mathcal{H}_t and does not depend on the coupling constant g , while \mathcal{H}_{Pt} is defined as \mathcal{H}_t but contains a kinematical factor depending on momenta of particle involved.

The resulting RGPEP equation has the form,

$$\mathcal{H}'_t = [[\mathcal{H}_f, \mathcal{H}_{Pt}], \mathcal{H}_t]. \quad (2.47)$$

Constructing an effective Hamiltonian using RGPEP amounts to solving this equation.

In general, the solution of the RGPEP equation is a non-trivial task, and a perturbative expansion of the effective Hamiltonian is used, expressing \mathcal{H}_t as a power series of the coupling constant g ,

$$\mathcal{H}_t = \sum_{n=0}^{\infty} g^n \mathcal{H}_{tn} = \mathcal{H}_0 + g \mathcal{H}_{t1} + g^2 \mathcal{H}_{t2} + g^3 \mathcal{H}_{t3} + g^4 \mathcal{H}_{t4} + \dots \quad (2.48)$$

Substituting into the RGPEP equation, and collecting terms order by order in g , the following system of coupled first-order differential equations is obtained,

$$\mathcal{H}'_0 = 0, \quad (2.49)$$

$$g \mathcal{H}'_{t1} = [[\mathcal{H}_0, g \mathcal{H}_{Pt1}], \mathcal{H}_0], \quad (2.50)$$

$$g^2 \mathcal{H}'_{t2} = [[\mathcal{H}_0, g^2 \mathcal{H}_{Pt2}], \mathcal{H}_0] + [[\mathcal{H}_0, g \mathcal{H}_{Pt1}], g \mathcal{H}_{t1}], \quad (2.51)$$

$$g^3 \mathcal{H}'_{t3} = [[\mathcal{H}_0, g^3 \mathcal{H}_{Pt3}], \mathcal{H}_0] + [[\mathcal{H}_0, g^2 \mathcal{H}_{Pt2}], g \mathcal{H}_{t1}] + [[\mathcal{H}_0, g \mathcal{H}_{Pt1}], g^2 \mathcal{H}_{t2}]. \quad (2.52)$$

\vdots

The order 0 term is trivially solvable from an initial condition, and the solution of the equation of order 1 will be an exponential of the parameter t times the initial condition \mathcal{H}_{01} . The 2nd order solution can be obtained from 1th order, and the 3rd order from the previous orders, and so on. At this point, the use of diagrams becomes crucial.

2.4.1 Regularization and Counterterms

In QCD, the bare Hamiltonian is ill-defined due to the presence of elements that contain ultraviolet (UV) divergences and infrared (IR) divergences [3, 19]. The UV divergences are produced in processes involving large momentum transfers, whereas the IR divergences occur in processes with ‘soft’ particles carrying small longitudinal momentum fractions, $x_{p/P} = p^+/P^+$, yielding zeros in denominators.

To deal with these divergences a regulating factor r is introduced in every interacting term. These factors make the interacting terms rapidly tend to zero, if the change in the transverse momentum of any gluon exceeds a certain cutoff parameter Δ , or if the change in longitudinal momentum of any gluon is greater than a cutoff parameter δ [20].

The particle operators are multiplied by the regulating factor,

$$r_{\Delta\delta}(k^\perp, x) = r_\Delta(k^\perp)r_\delta(x). \quad (2.53)$$

The transverse regulator factor, $r_\Delta(k^\perp)$ will ensure that UV processes are suppressed. And the longitudinal regulator factor $r_\delta(x)$ must verify a similar condition, preventing terms of the form $1/x$ or $1/x^2$ to blow up as x approaches 0.

The exact form of the regulator factors is not important for our purposes, as long as it verifies the condition, since it will be removed once we take the limit $\Delta \rightarrow \infty$ and $\delta \rightarrow 0$.

The counterterms are an additional term added to the initial or bare Hamiltonian \mathcal{H}_0 to deal with divergent integrals.

They are defined in a way, such that the coefficients of products of creation and annihilation operators in the effective theory for gluons of size s become independent of the regularization parameter Δ when the regularization in dynamics of gluons of size zero is being removed. The rest of the unknown parts of the counterterms are adjusted to respect the symmetries of the theory, and must match the predictions of the theory with the experimental results.

The distinction between regularization and counterterms may be confusing, but the regularization is a procedure to prevent the divergences that arise in the theory, while the counterterms are the terms added to the Hamiltonian to cancel the dependency on such regulators, so that after the cutoffs are removed, the effective Hamiltonian remains finite and regulator independent. Regularization is an essential first step in the renormalization process.

2.4.2 Order by order solutions.

The solution of the differential equations (2.50) to (2.52) and so on, without considering the RGPEP factors resulting from integration that would multiply each term.

$$\mathcal{H}_{t1} = f_t \mathcal{H}_{01} \tag{2.54}$$

$$\mathcal{H}_{t2} \sim \mathcal{H}_{02} + \mathcal{H}_{01} \mathcal{H}_{01} \tag{2.55}$$

$$\mathcal{H}_{t3} \sim \mathcal{H}_{03} + \mathcal{H}_{01} \mathcal{H}_{01} \mathcal{H}_{01} + (\mathcal{H}_{02} \mathcal{H}_{01} + \mathcal{H}_{01} \mathcal{H}_{02}) \tag{2.56}$$

$$\begin{aligned} \mathcal{H}_{t4} \sim & \mathcal{H}_{04} + \mathcal{H}_{01} \mathcal{H}_{01} \mathcal{H}_{01} \mathcal{H}_{01} + (\mathcal{H}_{02} \mathcal{H}_{01} \mathcal{H}_{01} + \mathcal{H}_{01} \mathcal{H}_{02} \mathcal{H}_{01} + \mathcal{H}_{01} \mathcal{H}_{01} \mathcal{H}_{02}) \\ & + (\mathcal{H}_{03} \mathcal{H}_{01} + \mathcal{H}_{01} \mathcal{H}_{03} + \mathcal{H}_{02} \mathcal{H}_{02}), \end{aligned} \tag{2.57}$$

\vdots

where f_t is a form factor that depends on the scale t which has the form of an exponential that results from the first-order equation. Such form factor suppresses the transition between states with different invariant mass.

Integrating order by order, additional factors are obtained. But they are ignored in this analysis and replaced by the symbol " \sim " to focus on structure resulting from the product of interactions.

This shows how an iterative process can be used to obtain the solution for each order.

The first-order diagrams are simply the canonical diagrams, with one power of g and denoted by \mathcal{H}_{01} .

As for the second order, they contain the canonical diagrams with power g^2 , and the counterterms, all together \mathcal{H}_{02} , and the product of 2 first-order diagrams.

The third order contains only the counterterms from the third order \mathcal{H}_{03} , the product of the first order, and second order canonical diagrams, as well as the product of exclusive first order diagrams.

3 Code implementation

The code is implemented in Python, but the principles of the method can be written in any programming language. The program is designed to be modular, and applicable to any other theory. These require changing the canonical diagrams. These modifications are beyond the scope of this work, and they are not presented here explicitly.

3.1 Diagram representation

Every term in the Hamiltonian can be identified with a diagram, according to the structure of the creation and annihilation operators present in it. The time order of the interaction is very important. In our convention, the time flows from right to left.

Each diagram will be composed of different elements:

- **External legs:** representation of the incoming and outgoing particles or the annihilation and creation operators, respectively. They determine the type of interaction that is being considered. (e.g. in figure 5, the connection of points [1, 2] or [3, 4] are external legs of the diagram.)
- **Internal legs:** represent the virtual particles that are exchanged during the process, or the intermediate creation and annihilation operators that are eliminated in the normal-ordering process. These creation and annihilation operators are not present in the effective Hamiltonian. (e.g. in figure 5, the 2 connection from [2, 3] are the internal legs of the diagram.)
- **Vertices:** points where interactions between particles occur, the number of vertices in a diagram indicates the order at which the diagram is contributing. (e.g. in figure 5, the points 1, 2, ... are the vertices of the diagram.)
- **Loops:** closed paths in the diagrams, formed by the internal legs. In general, they are divergent terms. Example in figure 5.

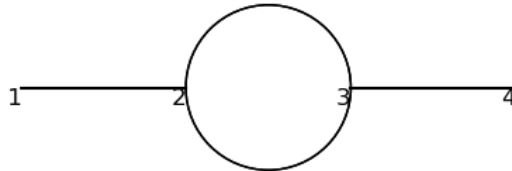


Figure 5: Example of a loop in a diagram, formed by the internal legs.

- **Counterterms** additional terms added to the Hamiltonian to deal with the divergences produced during the process. These will be represented with a dot in the diagram.

Notice that the diagrams are different from the well-known Feynman diagrams [8]. The essential difference is the importance of the order of appearance of the interactions. Altering the order of the vertices in the diagram will produce a different interaction terms.

As another example, consider the diagrams in figure 6, this pair of diagrams are contributions to the three-gluon vertex (one gluon yielding two gluons), with the counterterm associated with it.

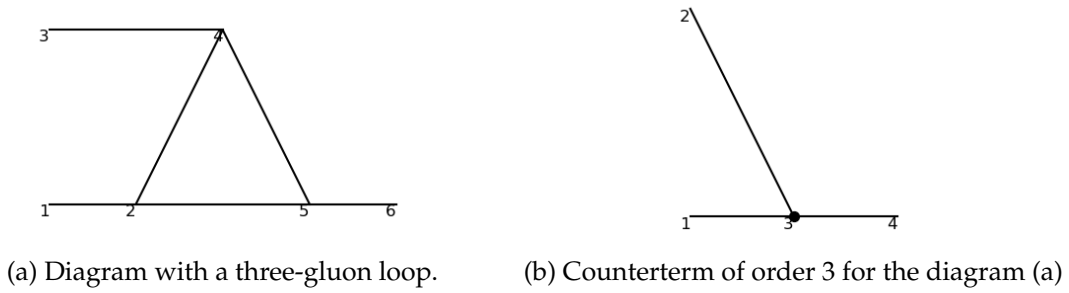


Figure 6: A example of a third order contribution to the process of three-gluon vertex, 1 gluon incoming and 2 gluons outgoing. (Outputs of the programs.)

Following the previous definitions, the diagram (figure 6a) represents a third order interaction with a three-gluon loop: 2 gluons are produced in the final state from one in the initial state. Due to the presence of a loop, the diagram is divergent, and a counterterm diagram is needed to deal with the divergence. This diagram is represented with a dot at the position of the loop, with the same external legs as the original diagram (figure 6).

3.2 Definition of diagrams

The diagrams are defined by 2 arrays,

- **Points:** arrays of dimension $N \times 2$, where N is the number of points in the diagram, each point is defined by its coordinates (x, y) .
- **Paths:** arrays of dimension $M \times N' \times 2$, where M is the number of different types of particles to consider in the theory, N' is the number of paths for each types of particle in the diagram, and 2 indicates the points to connect.

An example of the different elements can be seen in figure 7.

In the case of gluon interactions, although only 1 type of particle is present, the instantaneous interactions have to be considered. This is done by defining this interaction as a new type of virtual particle in the program.

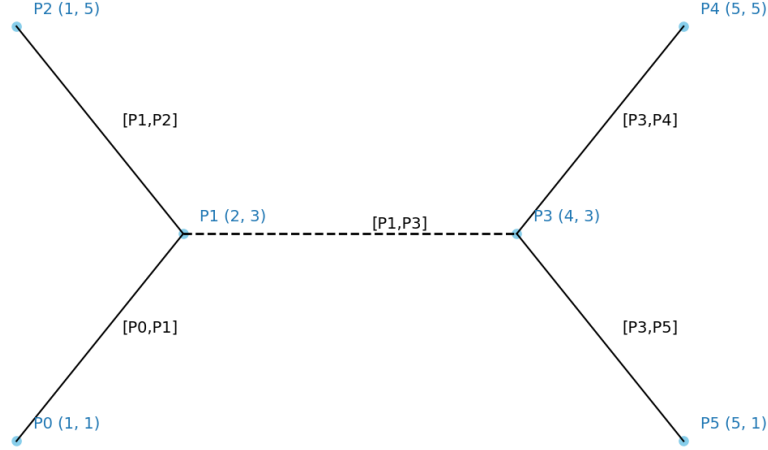


Figure 7: Representation of a diagram as a graph, where the blue points are the N points defined in the program, the different line-style represent the different types of particles M , and the labels associated with each line the N' connections for each type of particle.

3.3 Order by order procedure

To calculate the diagram representing a certain order-term, the code follows the procedure described in Section 2.4.2. Having the canonical diagrams as an input, the program aims to obtain all possible diagrams of such order that contribute to a certain effective interaction, and discards those diagrams, with different structure.

The program follows a recursive procedure, where the diagrams of order n are obtained from the diagrams of order lower orders, in a process that can be outlines as follows,

1. Start with the canonical diagrams of order 1 and 2.
2. For each order n , do the following,
 - (a) Generate all possible combinations of diagrams of lower orders, that sum to the order n .
 - (b) For each combination, check if it is a valid diagram ⁶ for the type of interaction being considered.
 - (c) If it is a valid diagram, add it to the list of diagrams for order n .
3. After generating all the diagrams of order n , check for equivalent diagrams, and add their contributions to the list of diagrams.
4. Check for loops, and add the counterterms for each order and process to the list of diagrams,
5. Repeat the process for the next order, until the desired order is reached.

⁶A 'valid' diagram here means that the external legs of the combined diagram match the intended process. For instance, if we are interested in the $1 \rightarrow 2$ gluon process, any combination that results in a different incoming/outgoing particle count would be discarded.

The step 3 is fundamental in order to reduce the number of diagrams that needs to be used to calculate the next order. This procedure is the most time-consuming process of the program, needing a search algorithm to find the equivalent diagrams, meaning that as the order increases, the number of diagrams increases exponentially, and the time to find the equivalent diagrams increases exponentially too.

To understand the process, let's consider the first iteration of the program, to calculate the diagrams of order 2, starting from the canonical diagrams of order 1.

$$\begin{aligned} \mathcal{H}_{01} \mathcal{H}_{01} &= \left(\begin{array}{c} \diagup \quad \diagdown \\ \hline \end{array} + \begin{array}{c} \diagdown \quad \diagup \\ \hline \end{array} \right) \left(\begin{array}{c} \diagup \quad \diagdown \\ \hline \end{array} + \begin{array}{c} \diagdown \quad \diagup \\ \hline \end{array} \right) = \\ &= \left(\begin{array}{c} \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \hline \end{array} + \begin{array}{c} \diagup \quad \diagdown \quad \diagdown \quad \diagup \\ \hline \end{array} + \begin{array}{c} \diagdown \quad \diagup \quad \diagup \quad \diagdown \\ \hline \end{array} + \begin{array}{c} \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \hline \end{array} \right) \end{aligned}$$

Here each term will contribute at second-order to a different type of interaction. For instance, the first term will contribute to the process of 1 gluon going to 3 gluons, since one of the outgoing gluon from the second diagram will "connect" to the incoming gluon of the first diagram. Due to 2 possible connections, this term produces 2 equivalent diagrams.

$$\begin{array}{c} \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \hline \end{array} \rightarrow 2 \cdot \begin{array}{c} \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \hline \end{array}$$

Similar procedure is followed for both the second and fourth terms, producing similar results. It is in the third term where more possibilities arise, since now either one connection or two connections can be considered, producing 2 different diagrams, of multiplicity 2.

$$\begin{array}{c} \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \hline \end{array} \rightarrow 2 \cdot \begin{array}{c} \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \hline \end{array} + 4 \cdot \begin{array}{c} \diagdown \quad \diagup \quad \diagdown \quad \diagup \\ \hline \end{array}$$

The first diagram will produce a loop, and thus a counterterm will be added to the list of diagram, to cancel the divergence produced.

3.4 Applied to gluon interactions

Although the focus of this thesis is only gluons, the program can be adapted to consider new types of particles.

The instantaneous process considered as a new type of particle, need to respect the time evolution of the system, meaning that in the eyes of the program, since the x-coordinate is different, the instantaneous interaction is no longer considered to be instantaneous, but rather a process that happens in a certain time interval. But since the instantaneous interactions really encodes a vertex, no other vertices can be present during the instantaneous interaction, and the program will ensure that this is the case.

4 Diagrams obtained

In this section, we will present the diagrams obtained from the program. At each order, we will consider the most relevant types of interaction.

4.1 Order 2

The second order diagrams correspond to the canonical diagrams of order 2, plus the diagrams obtained from the combination of the canonical diagrams of order 1 with itself and counterterms, shown in figure 12.

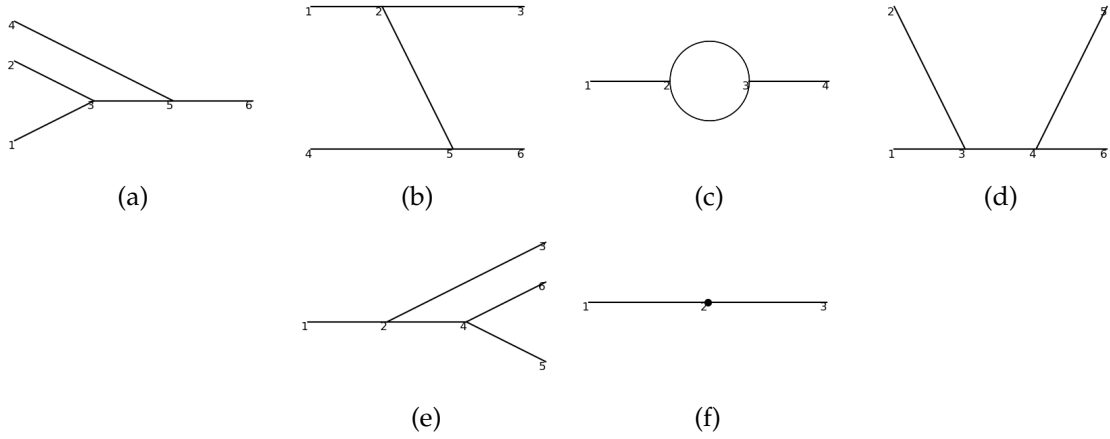
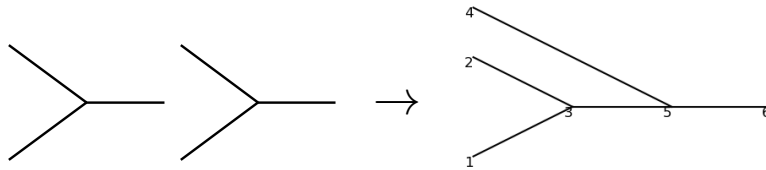
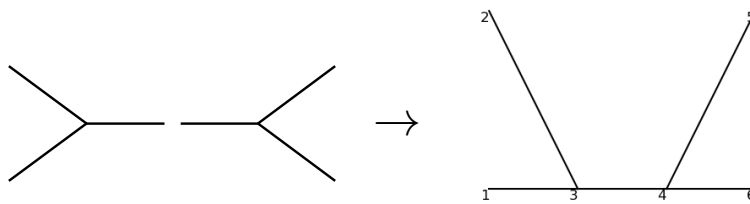


Figure 12: Some examples of diagrams of second order, obtained from the combination of the canonical diagrams of order 1. Fig. (f) represents second-order counterterm.

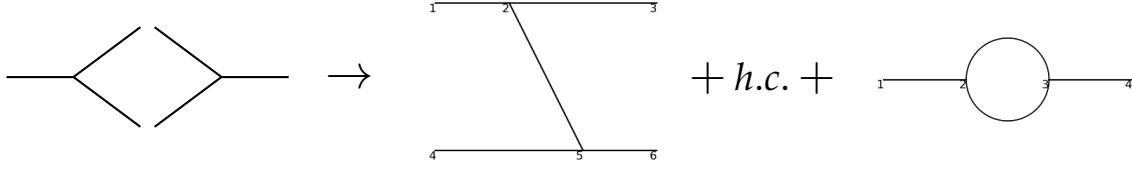
The diagram 12a is the combination of 2 1a diagrams, where one of the outgoing gluon from the first diagram becomes the incoming gluon of the second diagram.



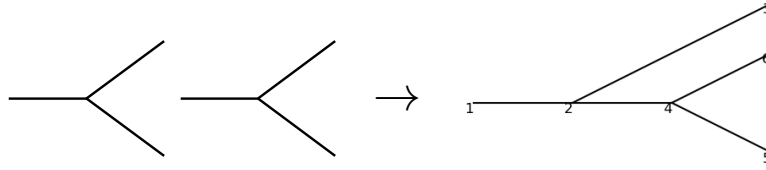
Similarly, the diagram 12e is the combination of 2 1b diagrams, the outgoing gluon of the first diagram is the one of the incoming gluon to the second diagram.



As for the diagrams 12b and 12c, both result from the combination of 1a and 1b diagrams, in that order, where the different diagrams are obtained depending on the number of connections between the incoming and outgoing gluons.



The diagram 12d is the combination of the 1b and 1a diagrams, where the outgoing gluon of the first diagram is the incoming gluon of the second diagram.



Finally, the diagram 12f is the counterterm associated with the second order diagrams, canceling the divergences that arises.

4.2 Three gluon vertex: 1 gluon to 2 gluons

Considering the process of 1 gluon going to 2 gluons, up till order 3, the diagrams obtained from the program are shown in the figures 17 and 18.

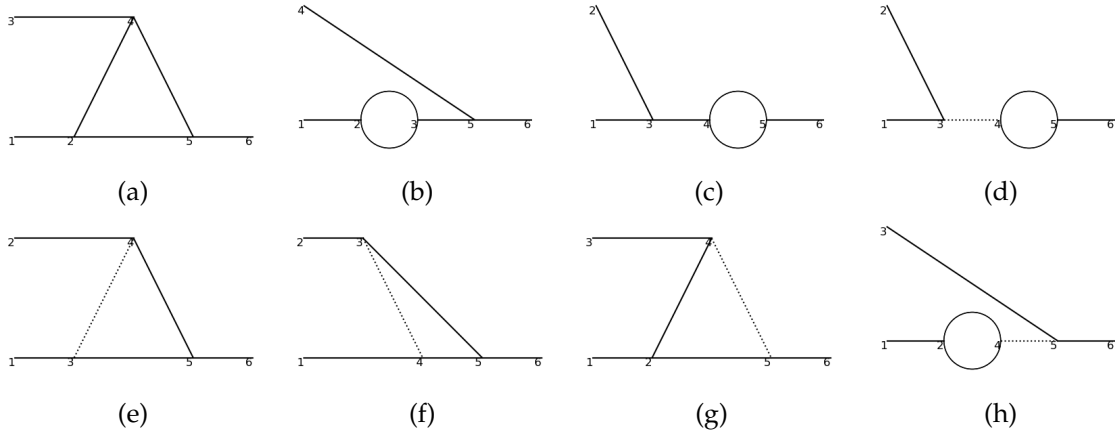


Figure 17: Diagrams of third order, contributing to the three-gluon vertex.

Depending on the types of particles in the process, we can deduce the origin of the different diagrams. Since the dotted lines are only present in the canonical diagrams of order 2.

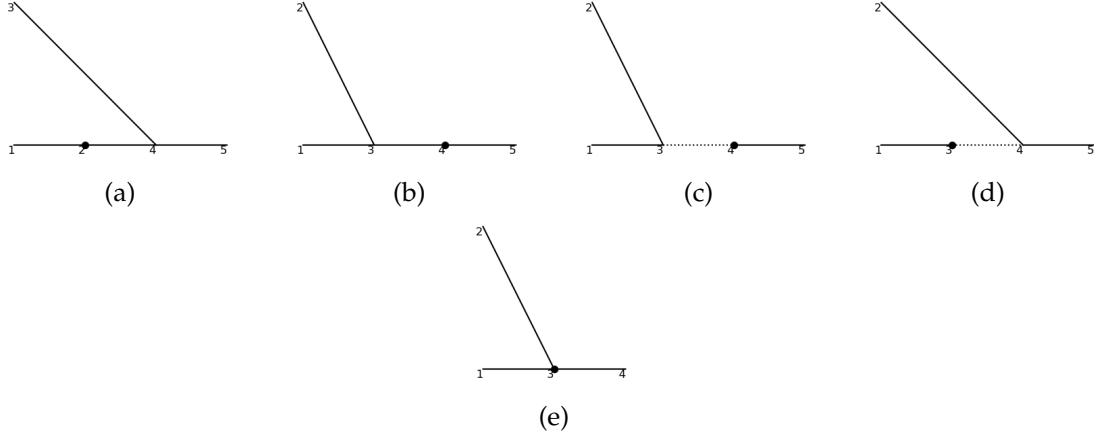


Figure 18: Third-order contributions containing counterterms [graphs (a) to (d)] and the third order counterterm [graph (e)].

Referring to the problems mentioned in Section 3.4, the diagrams with dotted lines are instantaneous interactions, but the program considers them as a new type of particle, there are some artifacts that arise from this approach. For instance, the diagrams 17e and 17f are actually the same diagram, due to instant process being instantaneous. For any other particle, these 2 diagrams would be different, due to the importance of the order in the interactions. Hence, the program keeps them different, to avoid the loss of generality.

Comparing with the 3rd order contribution diagrams in [3], the same diagrams for the three-gluon vertex are obtained, proving the validity of the program to reproduce the same results.

4.3 Self-energy: Gluon's effective mass

The self-energy describes the interaction of a gluon with itself, leading to modifications of the propagator and the effective mass of the gluon, such that at the infrared limit, the gluon mimics a massive particle. This is also reflected in or Hamiltonian formalism.

Each order of the effective Hamiltonian contains parts that contribute to different types of interactions,

$$\mathcal{H}_{nt} = \mathcal{H}_{nt}^{(1 \rightarrow 1)} + \mathcal{H}_{nt}^{(1 \rightarrow 2)} + \mathcal{H}_{nt}^{(2 \rightarrow 1)} + \dots \quad (4.1)$$

where $\mathcal{H}_{nt}^{(1 \rightarrow 1)}$ is the part of the Hamiltonian that contributes to the process of 1 gluon going to 1 gluon, $\mathcal{H}_{nt}^{(1 \rightarrow 2)}$ is the part that contributes to the process of 1 gluon going to 2 gluons, and so on.

This effective Hamiltonian can be expressed in terms of creation and annihilation operators, similar to Eqs.(2.38), as follows,

$$\mathcal{H}_{nt}^{(1 \rightarrow 1)} = \int [k] g^n \Sigma_t^{(n)}(k) a_t^\dagger(k) a_t(k), \quad (4.2)$$

where $\Sigma_t^{(n)}(k)$ is the self-energy correction at order n for the gluon self-energy. Comparing with the expression for the kinetic energy of the gluon, Eq. (4.2) introduces a correction, obtaining an effective kinetic energy, where $\Sigma_t^{(n)}(k)$ is interpreted as a mass-like term,

$$m_{nt}^2(k) = g^n \Sigma_t^{(n)}(k). \quad (4.3)$$

This way to study the self-energy of the gluon, we need to focus on the part of the Hamiltonian that contributes to the process of 1 gluon going to 1 gluon,

$$\mathcal{H}_t^{(1 \rightarrow 1)} = \mathcal{H}_{2t}^{(1 \rightarrow 1)} + \mathcal{H}_{4t}^{(1 \rightarrow 1)} + \dots \quad (4.4)$$

As for the effective kinetic term of the gluon, it verifies,

$$k_{eff}^- = \frac{k^{\perp 2} + m_t^2(k)}{k^+}, \quad (4.5)$$

with $m_t^2(k)$ being the effective mass considering all contributions from the expansion,

$$m_t^2(k) = g^2 \Sigma_t^{(2)}(k) + g^4 \Sigma_t^{(4)}(k) + g^6 \Sigma_t^{(6)}(k) + \dots \quad (4.6)$$

Then, it is in our best interest to obtain all the diagrams at each order that contribute to the gluon's self-energy.

At order 2, the diagram that contributes to the gluon's self-energy is presented in figure 12c and 12f. At order 4, the diagrams that contribute to the gluon's self-energy are shown in figure 19.

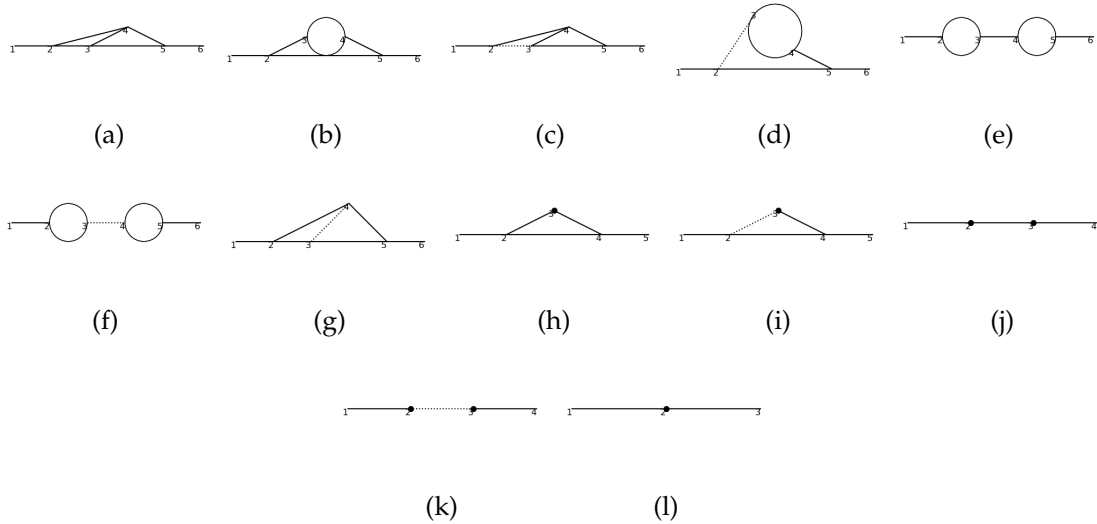


Figure 19: Diagrams of fourth order, contributing to the gluon's self-energy, with (h)-(k) diagrams with counterterms of order 2, and (l) the counterterm of order 4.

This thesis focuses on the generation of the diagrams, and thus we will not consider any calculation beyond this analysis, since they are far from the scope of this work. However, these possess a visual starting point for future calculations.

4.4 Bound states: Glueballs

Glueballs are color-singlet bound states of 2 or more interacting gluons, unlike mesons and baryons, which involve quarks and antiquarks, glueballs are composed solely of gluons. The existence of glueballs is predicted as a consequence of the non-abelian nature of QCD, where gluons interact strongly enough with each other to become dynamically confined. However, they are not confirmed experimentally nowadays. A deep theoretical understanding of their dynamic structure is welcomed.

The two to two gluon interaction is the simplest case of a glueball, and it can be obtained from the program by considering the process of 2 gluons going to 2 gluons. The diagrams obtained from the program are shown in figure 20.

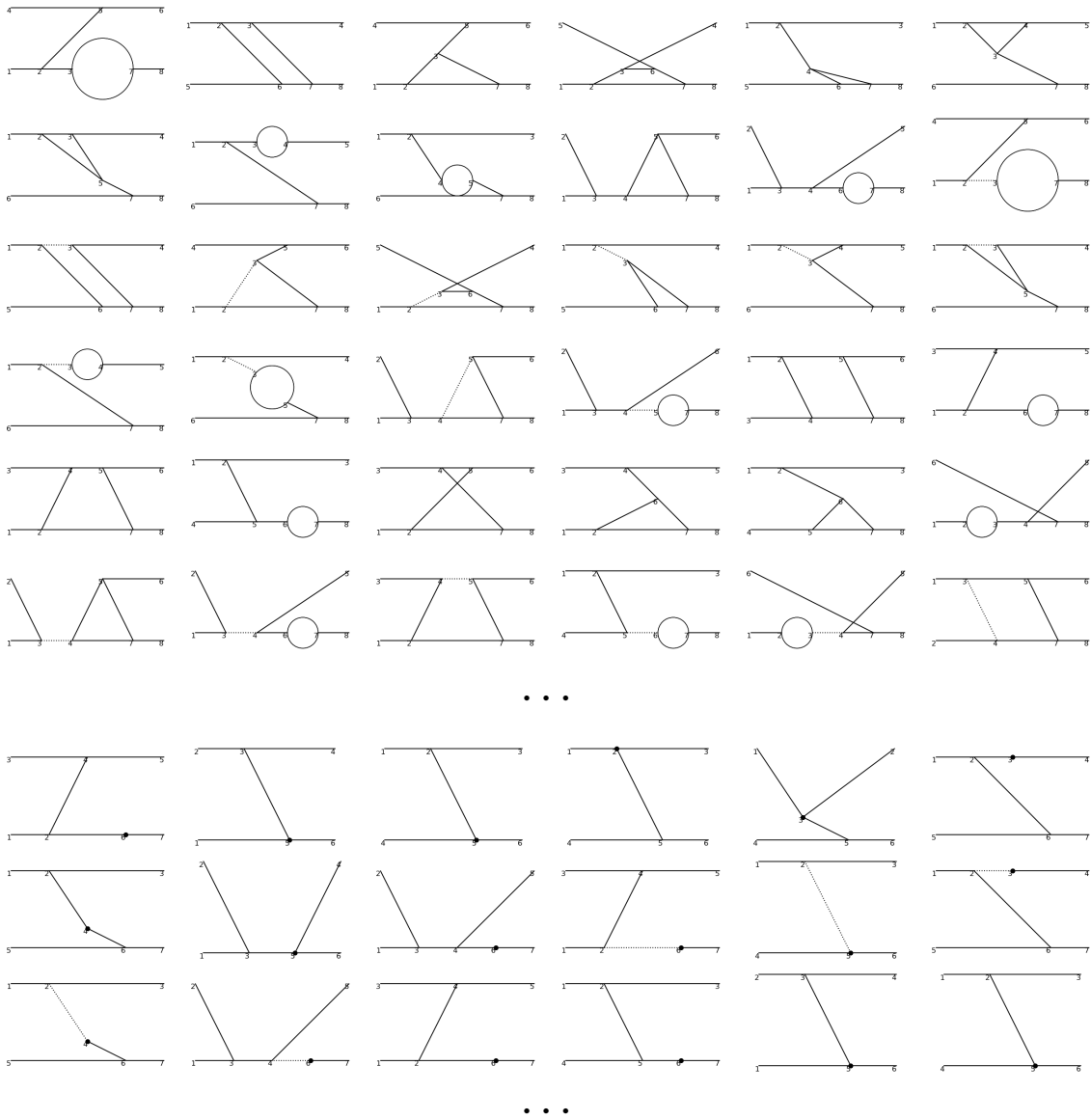


Figure 20: Some diagrams of fourth order, contributing to the process of 2 gluons going to 2 gluons.

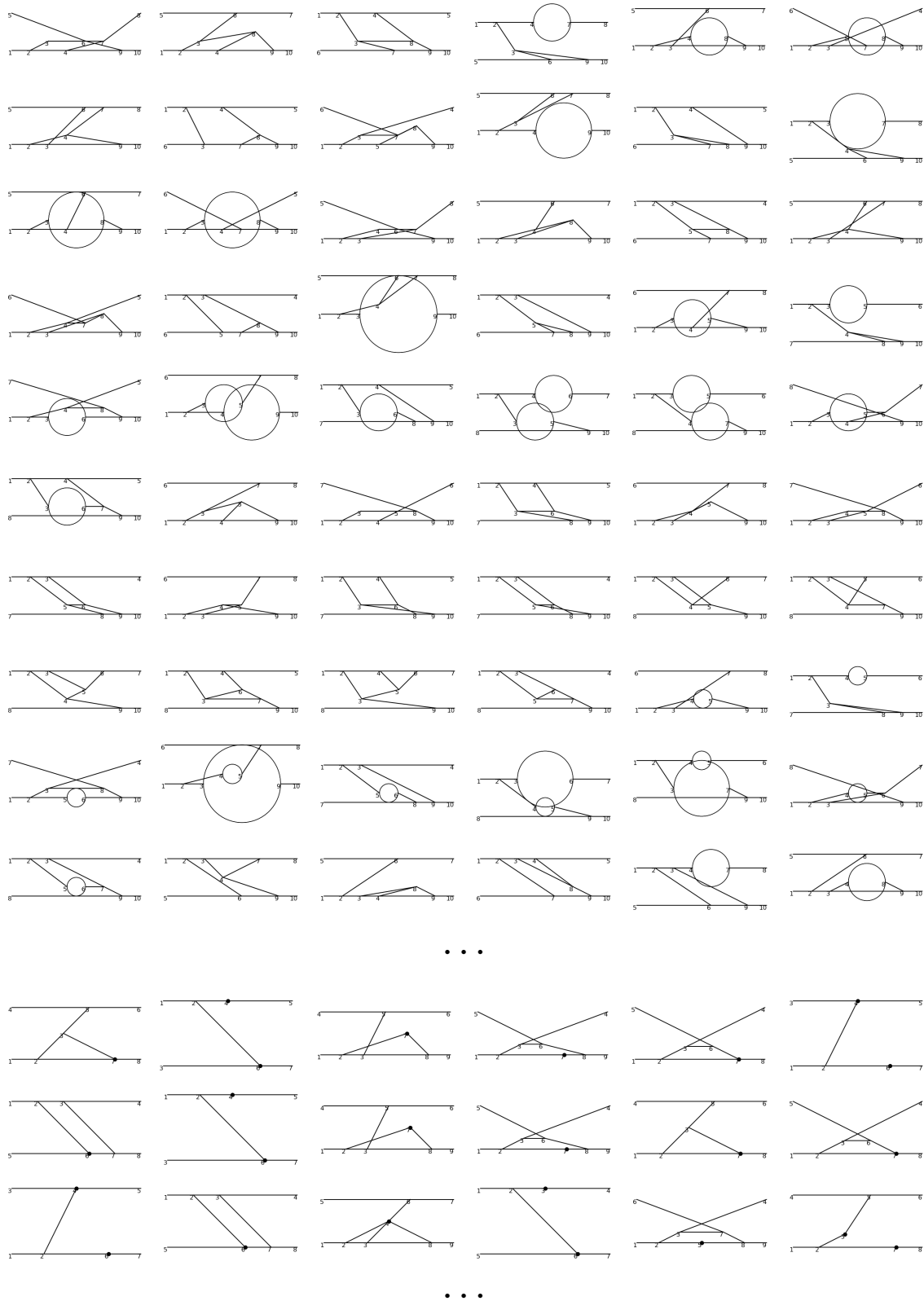


Figure 21: Some diagrams of sixth order, contributing to the process of 2 gluons going to 2 gluons.

4.5 Program performance

The program has been tested with orders up to sixth, and the results are shown in table 1.

Order	Types of diagrams	Computational time (s)
2	16	0.150
3	76	0.198
4	612	1.166
5	5871	10.935
6	65000	157.121

Table 1: Number of diagrams for all possible interactions, obtained by the program at each order, and the computational time taken at each order.

The table 1 shows the number of types of diagrams obtained by the program increases exponentially with the perturbative order, this exponential growth (Figs. 22, 23) the linearity in the logarithmic scale reflects the combinatorial explosion typical in perturbation theory.

The computational time also increases sharply, confirming that the diagram generation and evaluation becomes significantly more complex at higher orders.

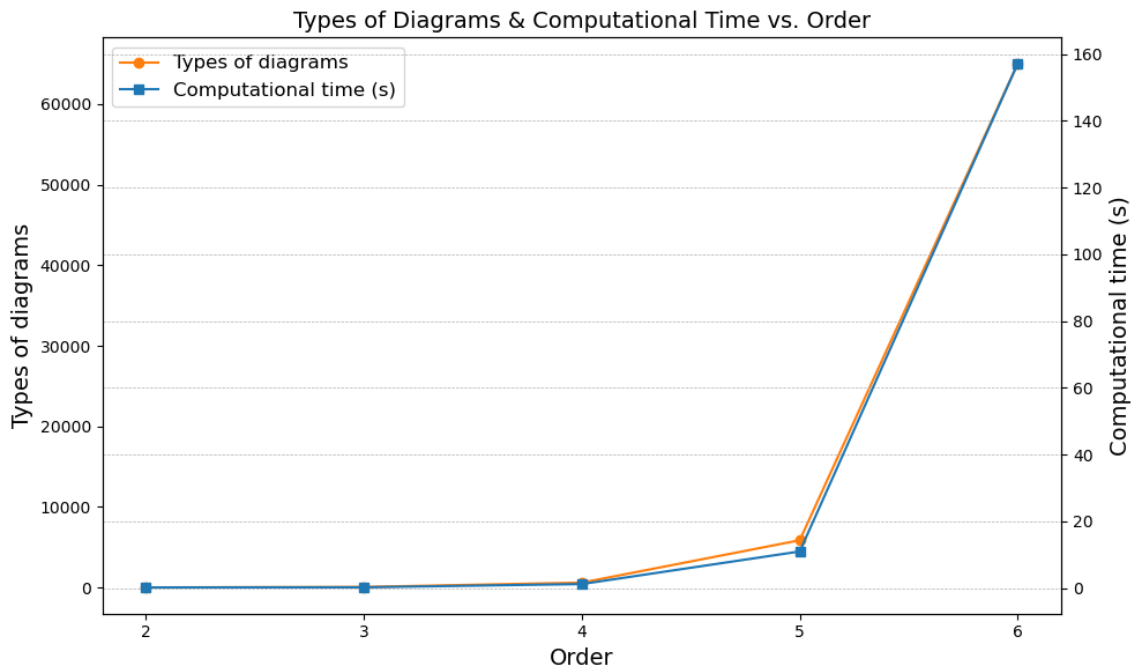


Figure 22: Representation of the types of diagrams with the computational time taken at each order.

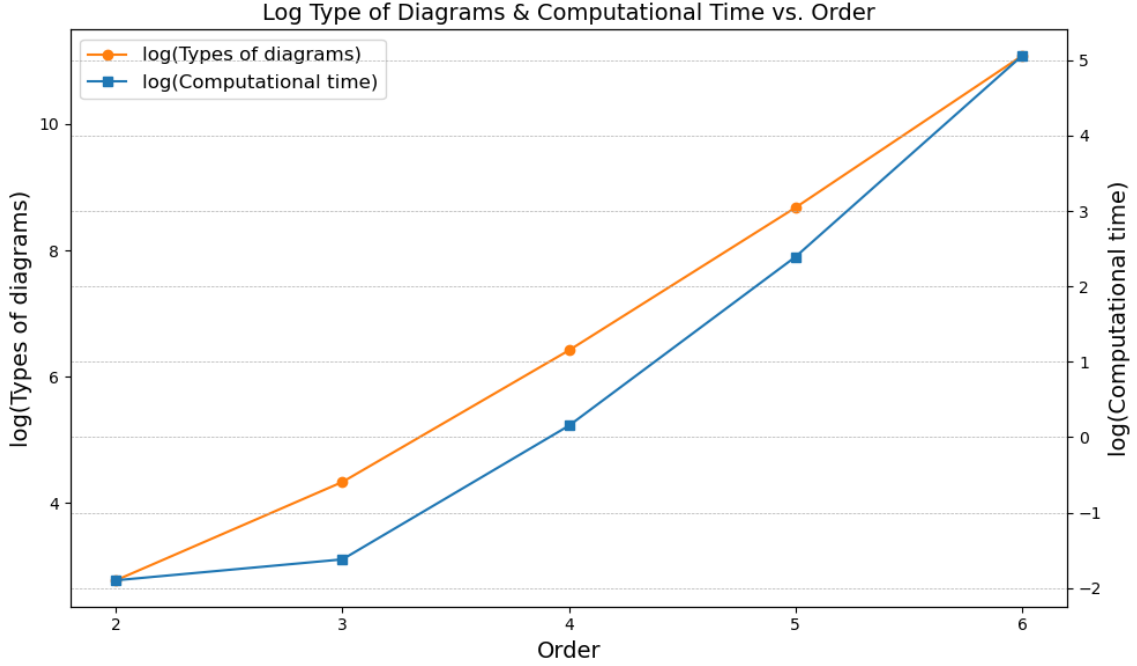


Figure 23: Log representation of the types of diagrams with the computational time taken at each order. The exponential growth of the number of diagrams and the computational time is more evident in this representation.

At lower orders (2 and 3), the overhead in the simulation breaks the exponential tendency, this is due to the intrinsic time necessary to run the code. But the simulation time is minimal and manageable, around (0.2s), showing the program is efficient for small systems or exploratory purposes.

The jump from 10.935s to 157.121s may reflect not only the increased number of diagrams, but also inefficiencies, such as: diagram redundancy checks, memory allocations or other computational overheads. A possible optimization could be to implement parallel processing or more efficient data structures to handle the growing complexity, which would help to reduce the computational time at higher orders. Other possible optimization could be avoiding the generation of diagrams that are not needed for the process considered, which would be relevant for higher orders.

5 Conclusions and future work

In this thesis, we presented a program to obtain diagram products in perturbative expansions. We illustrated it with an example of gluon interactions in the context of RGPEP. The program is modular and can be adapted to other theories by changing the canonical diagrams and the types of particles considered. It is, however, specific for time-ordered perturbation theory in the Hamiltonian formalism.

First, we have presented the RGPEP, and the framework necessary to understand the renormalization procedure, and the perturbative expansion of the Hamiltonian solution. Secondly, we explained the specific case of gluons self-interactions, within the theory of QCD, and the canonical Hamiltonian that describes the theory.

Then, we presented the program that implements the RGPEP, the definition of the diagrams in the program, how it is able to obtain the higher-order diagrams starting from the canonical diagrams, and using the order by order procedure described in section 2.4.2.

To check the correctness of the code, we tested it on the three-gluon vertex, obtaining the third-order diagrams and the corresponding counterterms to cancel the divergences produced in the process. The program was able to reproduce the diagrams obtained in previous works [3], proving enough confidence to proceed with higher-order diagrams in the perturbative expansion of the Hamiltonian.

We presented the gluon's self-energy, and showed how the program is able to obtain the diagrams that contribute to the effective mass of the gluon, an important object of study in QCD.

Another interesting case is the bound state. Using the program, we were able to obtain the diagrams that contribute to the process of two gluons going to two gluons, which is the simplest case of a glueball, showing the diagrams up to sixth order. The program is able to obtain higher-order diagrams, but the number of diagrams increases exponentially with perturbative order, making it impossible to show all the diagrams in this document.

Finally, we presented the performance of the program, showing the number of diagrams obtained at each order and the computational time required to obtain them. The results show that the number of diagrams increases exponentially with the perturbative order, and the computational time also increases sharply, confirming that the diagram generation and evaluation become significantly more complex at higher orders. The program is available in a public repository [1].

The program can be further developed in several interesting and useful ways, and there are numerous improvements that can be made to optimize the diagram-generation process. For instance, one of the main issue to address is the counting of the diagrams, since the program is able to obtain the diagrams, but it does not yet output the symmetry factor, due to complexities involved in the factors associated with the canonical diagrams, and counterterms.

As future work, we plan to fix the issues mentioned above, and to implement the program with other theories, and more types of particles, particularly consid-

ering the quarks and antiquarks, in the general case of QCD.

6 Conclusiones y trabajo futuro

En este trabajo, hemos presentado un programa para obtener productos de diagramas en expansiones perturbativas, en un formalismo hamiltoniano, ilustrando con un ejemplo de interacciones de gluones en el contexto del RGPEP. El programa es modular y puede ser adaptado a otras teorías, cambiando los diagramas canónicos y los tipos de partículas consideradas. Es, sin embargo, específico para la teoría de perturbaciones en orden temporal en el formalismo Hamiltoniano.

Primero, hemos presentado el marco teórico necesario para entender el procedimiento de renormalización, y la expansión perturbativa de la solución de la ecuación de flujo. En segundo lugar, explicamos el caso específico de la interacción de los gluones, dentro de la teoría de QCD y el Hamiltoniano canónico que describe la teoría.

Luego, presentamos el programa que implementa el RGPEP, la definición de los diagramas en el programa, cómo es capaz de obtener los diagramas de orden superior, comenzando desde los diagramas canónicos, y utilizando el procedimiento orden a orden descrito en la sección 2.4.2.

Para comprobar la validez del código, estudiamos el vértice de tres gluones, obteniendo los diagramas de tercer orden, y los correspondientes contratérminos para cancelar las divergencias producidas en el proceso. El programa fue capaz de reproducir los diagramas obtenidos en trabajos anteriores [3], ofreciendo suficiente confianza para obtener diagramas de orden superior en la expansión perturbativa del Hamiltoniano.

Presentamos la autoenergía del gluón y cómo el programa es capaz de obtener los diagramas que contribuyen a la masa efectiva del gluón, un objeto de estudio importante en QCD.

Otro caso interesante es el de los estados ligados. Usando el programa, pudimos obtener los diagramas que contribuyen al proceso de dos gluones yendo a dos gluones, que es el caso más simple de un glueball, hasta sexto orden. El programa es capaz de obtener los diagramas de orden superior, pero el número de diagramas aumenta exponencialmente con el orden perturbativo, haciendo imposible mostrar todos los diagramas en este documento.

Finalmente, presentamos el rendimiento del programa, mostrando el número de diagramas obtenidos en cada orden y el tiempo computacional tomado para obtenerlos. Los resultados muestran que el número de diagramas aumenta exponencialmente con el orden perturbativo y el tiempo computacional también aumenta bruscamente, confirmando que la generación y evaluación de diagramas se vuelve significativamente más compleja a ordenes superiores. El programa está disponible en un repositorio público [1].

El código puede ser desarrollado más allá de lo presentado en este trabajo, y hay algunas mejoras que se pueden hacer para optimizar el proceso de obtención de los diagramas. Por ejemplo, uno de los principales problemas a resolver es el

conteo de los diagramas, el programa es capaz de obtener los diagramas, pero no produce el factor de simetría todavía, debido a las complejidades involucradas en los factores asociados a los diagramas canónicos, y a los contratérminos.

Como trabajo futuro, planeamos implementar los desarrollos mencionados anteriormente y extenderlo a otras teorías y tipos de partículas, particularmente considerando quarks y antiquarks en el caso general de QCD.

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