

Quantum integration of decay rates at second order in perturbation theory

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We present the first quantum computation of a total decay rate in high-energy physics at second order in perturbative quantum field theory. This work underscores the confluence of two recent cutting-edge advances. On the one hand, the quantum integration algorithm Quantum Fourier Iterative Amplitude Estimation (QFIAE), which efficiently decomposes the target function into its Fourier series through a quantum neural network before quantumly integrating the corresponding Fourier components. On the other hand, causal unitarity in the loop-tree duality (LTD), which exploits the causal properties of vacuum amplitudes in LTD to coherently generate all contributions with different numbers of final-state particles to a scattering or decay process, leading to singularity-free integrands that are well suited for Fourier decomposition. We test the performance of the quantum algorithm with benchmark decay rates in a quantum simulator and in quantum hardware, and find accurate theoretical predictions in both settings.

I. INTRODUCTION

The interplay between high-energy physics and quantum computing represents a promising frontier for advancing our understanding of fundamental concepts and improving computational techniques. High-energy physics requires complex theoretical calculations to predict with high accuracy cross sections and decay rates, which are essential for understanding the behavior of elementary particles at quantum scales and for validating theoretical models in quantum field theory [1]. These complex calculations often challenge classical computational methods. Quantum computing, with its inherent ability to leverage the principles of quantum mechanics, offers a novel approach to successfully addressing these challenges [2–4]. The applications of quantum computing in this field include jet identification and clustering [5–8], parton density determination and integration [9, 10], parton shower simulation [11], anomaly detection [12–14], elementary particle process integration [15], data classification [16] and multiloop Feynman diagram causal structure [17, 18].

In particle physics, Feynman diagrams and scattering amplitudes from perturbative quantum field theory are essential tools for predicting the transition probabilities between particle states at high-energy colliders, such as the CERN’s Large Hadron Collider. Loop Feynman diagrams represent interactions between particles that involve virtual quantum fluctuations, making them inherently complex. On the other hand, tree-level Feynman diagrams represent direct interactions between particles, and although they are apparently easier to evaluate, they are not exempt from difficulties. Traditional methods for evaluating Feynman diagrams and scattering amplitudes, and combining them to extract accurate theoretical predictions, while effective, are limited by their computational complexity and the resources required to perform, for exam-

ple, numerical integrations over the loop momenta and the phase space of the final states.

The loop-tree duality (LTD) framework [19–24] facilitates the evaluation of multiloop Feynman diagrams by decomposing them into tree-like objects, providing a structured approach to these computations where the fundamental physical principle of causality is manifest in the integrand representation [25–32]. We have recently proposed a novel approach based on LTD to efficiently recast perturbative theoretical predictions at high-energy colliders, the LTD causal unitarity [33, 34], where differential observables, cross sections and decay rates are assembled from the LTD representation of vacuum amplitudes, i.e. scattering amplitudes without external particles.

In Ref. [35, 36], we have also proposed a quantum integration algorithm, dubbed Quantum Fourier Iterative Amplitude Estimation (QFIAE), and in Ref. [37] we have applied this quantum integrator to the evaluation of infrared-safe scalar one-loop Feynman integrals.

By integrating quantum computing techniques into the LTD framework and harnessing the power of quantum integration, we expect a transformative approach that could lead to new insights and more efficient methodologies. Therefore, the aim of this work is going one step further and test the performance of QFIAE with physical decay rates at second order in perturbation theory or next-to-leading order (NLO). This requires the combination of one-loop with three-level contributions, where each of the contributions is individually singular and therefore numerically challenging, although the final prediction is finite. We base our approach on the LTD causal unitarity framework because the unified treatment of loop and three-level contributions leads to rather flat integrands, and therefore integrands that are more suitable for numerical integration, in particular, by Fourier decomposition.

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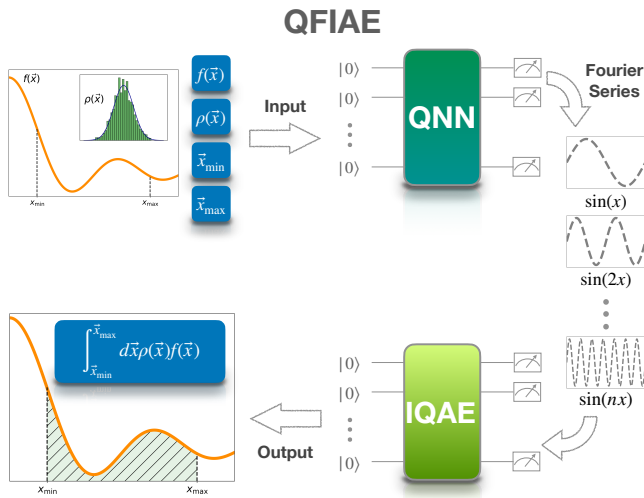


FIG. 1. Workflow of QFIAE. The input consists of the target function $f(\vec{x})$, the probability distribution $\rho(\vec{x})$, and the integration domain $\{x_{min}, x_{max}\}$. The QNN fits $f(\vec{x})$ and extracts its Fourier series from the quantum circuit. Next, IQAE estimates the integral for each trigonometric term in the Fourier series. Finally, these integrals are added with their corresponding coefficients to obtain the final integral result.

II. QUANTUM FOURIER ITERATIVE AMPLITUDE ESTIMATION

Quantum Fourier Iterative Amplitude Estimation (QFIAE) [35–37] is a quantum algorithm designed to efficiently integrate multidimensional functions. Its workflow is depicted in Fig. 1. QFIAE first decomposes the target function into its Fourier series using a Quantum Neural Network (QNN) via a data re-uploading approach [38–40]. Previous studies [38, 41] have demonstrated that an exponential data encoding results in the quantum model representing a truncated Fourier series. Following this first step, each trigonometric term of the Fourier series undergoes quantum integration using Iterative Quantum Amplitude Estimation (IQAE) [42], which is an efficient variant of Quantum Amplitude Estimation (QAE) [43].

The Fourier decomposition enables encoding the target function with minimal quantum arithmetic operations and also capitalizes on the quantum-friendly nature of the sine function for integration purposes. At the core of QFIAE lies the QNN, which provides a practical approach to preserving the potential quadratic speedup in the number of queries to the probability distribution function, which will be encoded into the amplification operator, offered by the Amplitude Amplification algorithm underlying in QAE, compared to other recently proposed quantum integration algorithms like Fourier Quantum Monte Carlo Integration (FQMCI) [44]. FQMCI, also employs Fourier decomposition to approximate the integrand and then individually estimate each component using QAE. However, FQMCI relies on assumptions about acquiring the Fourier coefficients, which may not always hold. Failure to meet these assumptions can nullify the potential quan-

tum speedup. The QNN, on the other hand, ensures a reliable quantum extraction of the Fourier coefficients.

The second critical aspect of QFIAE involves exploiting the advantages of IQAE over QAE. QAE estimates quantum state amplitudes using amplitude amplification, an extension of Grover’s algorithm [45], to enhance the likelihood of measuring the desired state over undesired states. However, QAE is constrained by its dependence on the resource-intensive Quantum Phase Estimation (QPE) subroutine [46], which entails operations deemed computationally expensive for current Noisy Intermediate Scale Quantum (NISQ) devices. This limitation threatens the anticipated quadratic advantage promised by QAE. IQAE addresses this challenge by replacing QPE with a classically efficient post-processing method, reducing the demands on qubits and quantum gates while preserving the asymptotic quadratic speedup.

III. LTD CAUSAL UNITARY AND DECAY RATES AT NLO

A vacuum amplitude in LTD, $\mathcal{A}_D^{(\Lambda)}$, where Λ is the number of primitive loop four-momenta, is obtained from its Feynman representation by integrating out through the Cauchy residue theorem one component of each primitive loop momenta [19, 20], typically the energy components, which results in replacing the Feynman propagators by causal propagators of the form [25]

$$\frac{1}{\lambda_{i_1 \dots i_m}} = \left(\sum_{s=1}^m q_{i_s,0}^{(+)} \right)^{-1}, \quad (1)$$

where $q_{i_s,0}^{(+)} = \sqrt{\mathbf{q}_{i_s}^2 + m_{i_s}^2 - i0}$ are the on-shell energies of the internal propagators, with \mathbf{q}_{i_s} the spatial components of the four-momenta and m_{i_s} their masses. The numerator of the vacuum amplitude in LTD is also a function of the on-shell energies and additionally of the internal masses. The factor $i0$ in the on-shell energies stems from the original infinitesimal complex prescription of the Feynman propagators. Loop vacuum amplitudes in the customary Feynman representations are functions in the Minkowski space of the loop four-momenta, while the integration domain of loop vacuum amplitudes in LTD is the Euclidean space of the loop three-momenta.

Each causal propagator, Eq. (1), involves a set of internal particles that divide the vacuum amplitude into two subamplitudes, with the momentum flow of all particles in the set aligned in the same direction, and each term in the vacuum amplitude is proportional to a product of causal propagators in which the momentum flow of the shared particles are also aligned in the same direction [26–31]. This picture is also analogous to selecting the acyclic configurations of a directed graph in graph theory [17, 18, 47]. In the limit where a causal propagator becomes singular, all the particles involved are set on shell. Therefore a natural procedure to generate all the interferences of scattering amplitudes with different numbers of final-state particles that are considered in the state-of-the-art approaches is to take residues on the causal propagators. This

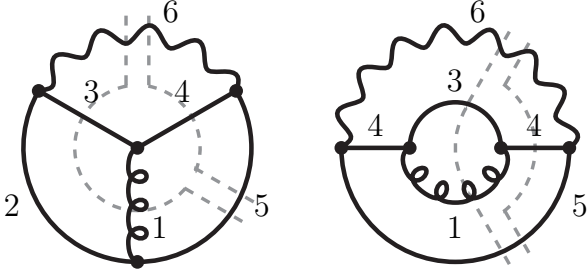


FIG. 2. Three-loop vacuum diagrams contributing to the decay $\gamma^* \rightarrow q\bar{q}(g)$ at NLO. The gray dashed lines represent phase-space residues, i.e. different final states. Similar diagrams contribute to the decays $H \rightarrow q\bar{q}(g)$ and $\Phi \rightarrow \phi\phi(\phi)$ by substituting the photon labeled 6 by a Higgs boson or a heavy scalar Φ ; and particles 1 to 5 by light scalars.

is the central idea of LTD causal unitary [33, 34]. The vacuum amplitude in LTD thus acts as a kernel amplitude, which generates all the final states contributing to a scattering or decay process from all possible residues on causal propagators.

As benchmark decay rates at NLO, we consider the decay of a heavy scalar into lighter scalars, and the decay of a Higgs boson or an off-shell photon into a pair of massive quarks and antiquarks. These processes have been implemented for a proof of concept of LTD causal unitary in Ref. [34], where classical integration methods were used to predict the total decay rates. We refer to Ref. [34] for a detailed presentation of the expressions used in the numerical implementation. The vacuum diagrams that contribute to the decay $\gamma^* \rightarrow q\bar{q}(g)$ are shown in Fig. 2. Similar vacuum diagrams describe the other two decay processes considered.

The vacuum diagrams in Fig. 2 contribute to a vacuum amplitude that in LTD depends on three loop three-momenta, $\{\ell_1, \ell_2, \ell_3\}$. The three-momenta of the internal propagators read

$$\begin{aligned} \mathbf{q}_1 &= \ell_1 + \ell_2, & \mathbf{q}_2 &= \ell_1 + \ell_3, & \mathbf{q}_3 &= \ell_1, \\ \mathbf{q}_4 &= \ell_2, & \mathbf{q}_5 &= \ell_2 - \ell_3, & \mathbf{q}_6 &= \ell_3, \end{aligned} \quad (2)$$

and the corresponding on-shell energies are given by $q_{i,0}^{(+)} = \sqrt{\mathbf{q}_i^2 + m_i^2} - i0$. We work in the rest frame of the decaying particle, where $\ell_3 = \mathbf{0}$. Therefore, the unintegrated decay rate is a function of the remaining three-momenta, ℓ_1 and ℓ_2 , through the on-shell energies.

The differential decay rate of a particle a at NLO takes the form

$$\begin{aligned} d\Gamma_a^{(1)} &= \frac{d\Phi_{\ell_1\ell_2}}{2\sqrt{s}} \left[\left(\mathcal{A}_D^{(3,a)}(456) \tilde{\Delta}_{45\bar{6}} + \mathcal{A}_D^{(3,a)}(1356) \tilde{\Delta}_{135\bar{6}} \right) \right. \\ &\quad \left. + (5 \leftrightarrow 2, 4 \leftrightarrow 3) \right], \end{aligned} \quad (3)$$

where $\mathcal{A}_D^{(3,a)}(456)$ and $\mathcal{A}_D^{(3,a)}(1356)$ are the phase-space residues of the vacuum amplitude in LTD, i.e. they are obtained from the residue on the corresponding causal propagators. They represent the perturbative quantum fluctuations at

one-loop with two final-state particles, and at tree-level with three final-state particles, respectively. For example, for the decay of a heavy scalar Φ into lighter scalars, the phase-space residues are

$$\begin{aligned} \mathcal{A}_D^{(3,\Phi)}(456) &= \frac{g_\Phi^{(1)} m_\Phi^2}{x_{12345}} \left(L_{234\bar{5},125}^{13\bar{4}} + L_{234\bar{5},134}^{12\bar{5}} + L_{134,125}^{23\bar{4}\bar{5}} \right), \\ \mathcal{A}_D^{(3,\Phi)}(1356) &= \frac{g_\Phi^{(1)} m_\Phi^2}{x_{135}} \left(\frac{1}{\lambda_{13\bar{4}} \lambda_{134} \lambda_{12\bar{5}} \lambda_{125}} \right), \end{aligned} \quad (4)$$

where $g_\Phi^{(1)}$ encodes the interaction couplings, the factor $x_{i_1 \dots i_n} = \prod_{s=1}^n 2q_{i_s,0}^{(+)}$ is the product of the corresponding on-shell energies and $L_{j,k}^i = \lambda_i^{-1} (\lambda_j^{-1} + \lambda_k^{-1})$, with

$$\lambda_{i_1 \dots i_r \bar{i}_{r+1} \dots \bar{i}_n} = \lambda_{i_1 \dots i_r} - \lambda_{i_{r+1} \dots i_n}. \quad (5)$$

The integration measure is written in terms of two loop three-momenta

$$d\Phi_{\ell_1\ell_2} = \prod_{j=1}^2 \frac{d^3\ell_j}{(2\pi)^3}, \quad (6)$$

i.e. six integration variables. However, each term in Eq. (3) must satisfy energy conservation, which is encoded in

$$\tilde{\Delta}_{i_1 \dots i_n \bar{a}} = 2\pi \delta(\lambda_{i_1 \dots i_n \bar{a}}), \quad (7)$$

and the decay is isotropic in the rest frame of the decaying particle. As a result, the decay rate depends on two independent integration variables; a polar angle, which is usually parametrized as $\cos\theta = 1 - 2v$, with $v \in [0, 1]$, and the modulus of one of the loop three-momenta, mapped from $[0, \infty)$ to the finite interval $[0, 1)$ in the numerical implementation.

The most important feature of Eq. (3) is that loop and tree-level contributions, i.e. contributions with different numbers of final-state particles, are treated simultaneously under the same integration measure. This property guarantees the local cancellation of singularities arising in the state-of-the-art approach, and thus avoids having to perform intermediate calculations in arbitrary space-time dimensions [48, 49]. In addition, the resulting integrand is flatter than in other approaches, allowing for a much faster and more efficient numerical implementation.

IV. QUANTUM INTEGRATION OF NLO DECAY RATES

In this section, we apply the quantum integration algorithm QFIAE to estimate the total decay rate at NLO of the decay processes presented in Section III. The main challenge of this quantum implementation is in making the QNN to fit well the differential decay rate function. To address this problem we present a QNN with a general-purpose Ansatz, see Fig. 5, which contains enough entanglement and free parameters to permit a high expressibility that enables the correct solution of the regression problem.

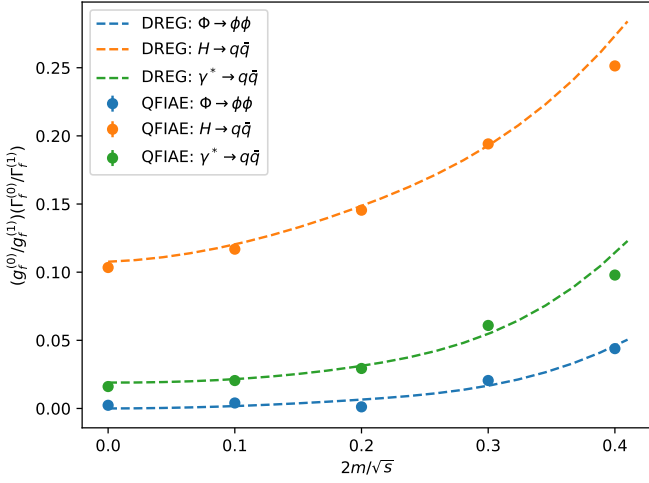


FIG. 3. Quantum-integrated decay rates in a quantum simulator for the three decay processes $H \rightarrow q\bar{q}(g)$, $\gamma^* \rightarrow q\bar{q}(g)$ and $\Phi \rightarrow \phi\phi(\phi)$ at NLO as a function of the final state mass, using QFIAE and LTD causal unitary. The dashed lines are the theoretical predictions in dimensional regularization. The parameters used in the quantum implementation are: $max_steps = 15000$, $step_size = 0.001$, $layers = n_{Fourier} = 20$, $n_{qubits} = 6$ for the QNN and $n_{qubits} = 5$, $n_{shots} = 10^3$, $\epsilon = 0.01$, $\alpha = 0.05$ for the IQAE module.

We utilize PennyLane [50] to construct and train the QNN. The IQAE module is implemented with `Qibo` [51] on quantum simulators, Fig. 3, and with `Qiskit` [52] on a real hardware, Fig. 4. In particular, this module is executed on the 27-qubit IBMQ superconducting device *ibmq_mumbai*. The QNN architecture, which is displayed in Fig. 5, consists of a 6-qubit quantum circuit with a specific Ansatz repeated n_{layers} times within the circuit. This Ansatz comprises two key components: a variational part with trainable parameters built using `qml.StronglyEntanglingLayers`, and an encoding block for two variables. Each variable is encoded three times in parallel across the 6 qubits using `qml.AngleEmbedding`.

After making our QNN to accurately mimic the target function, we extract the Fourier series and feed the IQAE subroutine with it. For the IQAE module, we design a quantum circuit with a relatively low depth and low number of qubits that opens up the possibility to be executed on current quantum computers. We also implement error mitigation techniques to obtain the desirable results. In particular, to mitigate quantum noise during execution, we utilized a pulse-efficient transpilation technique [53], which effectively reduces the number of two-qubit gates by leveraging the hardware-native cross-resonance interaction. Additionally, we applied the error suppression technique Dynamical Decoupling (DD) within the circuit execution and the error mitigation technique Zero Noise Extrapolation (ZNE) to the output, using the `Qiskit Runtime Estimator primitive` [54].

The results presented in Fig. 3 and 4 show a relatively small deviation with respect to their corresponding analytical values in the standard dimensional regularization. In particular, in

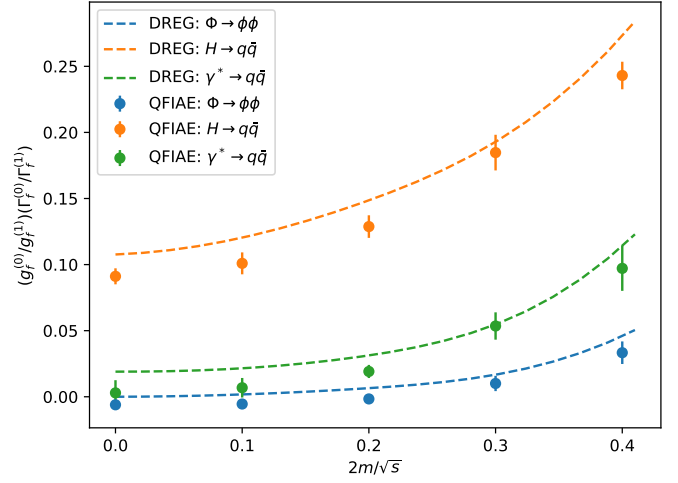


FIG. 4. Quantum-integrated decay rates in quantum simulator (hardware) for the QNN (IQAE) module of the QFIAE, for the three decay processes $H \rightarrow q\bar{q}(g)$, $\gamma^* \rightarrow q\bar{q}(g)$ and $\Phi \rightarrow \phi\phi(\phi)$ at NLO as a function of the final state mass, using QFIAE and LTD causal unitary. The dashed lines are the theoretical predictions in dimensional regularization. The parameters used in the quantum implementation are: $max_steps = 15000$, $step_size = 0.001$, $layers = n_{Fourier} = 20$, $n_{qubits} = 6$ for the QNN and $n_{qubits} = 5$, $n_{shots} = 10^3$, $\epsilon = 0.01$, $\alpha = 0.05$ for the IQAE module.

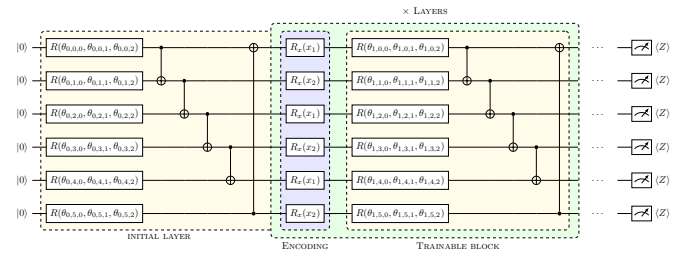


FIG. 5. Architecture of the QNN employed to fit a 2-dimensional function.

Fig. 4, one can notice that in comparison to Fig. 3 there's a systematic deviation in the value of the integrals introduced by the hardware noise and that is still not alleviated by the currently available error mitigation techniques applied. Nevertheless, most of the values are in agreement within the uncertainty bands with the expected values, so we consider that the results are quite satisfactory, taking into account the current limitations of real quantum hardware.

V. CONCLUSIONS

We have presented the first quantum computation of a total decay rate at second order in perturbative quantum field theory. Leveraging the loop-tree duality (LTD) framework, we have successfully combined loop and tree-level Feynman diagrams with a quantum algorithm on a quantum computer. This

methodological advancement is significant from the high-energy physics perspective, as it allows us to integrate a real process with potential for quantum speedup. While we do not claim to have achieved quantum speedup in this work, our results lay the groundwork for future explorations in this direction. From the perspective of quantum computing, our study marks a noteworthy achievement. By solving a relatively complicated regression problem using a Quantum Neural Network (QNN) on a realistic dataset, we found a good compromise between trainability and expressibility, a common challenge in quantum neural networks. Most of the results presented are in agreement with the expected values within the uncertainty bands. This demonstrates the potential of quantum computing to address complex, real-world problems and highlights the importance of continuing to push the boundaries of what quantum technology can achieve.

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