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Quantum simulation of colour in perturbative QCD

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ACAT conference 2024 (Stony Brook)
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Based on SciPost Phys. 15, 205 (2023)
with Mathieu Pellen

and ongoing work with Mathieu Pellen and Simon Williams

Outline

1. Introduction/motivation
2. Background
3. Quantum circuits for colour
 - Overview
 - Details
4. Results/validation
5. Outlook and summary



Outline

1. Introduction/motivation

- Why perturbative QCD?
- Why quantum computers?
- Why now?
- Proposed applications of quantum computing in high-energy physics

2. Background

3. Quantum circuits for colour

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Why perturbative QCD? (1)

Particle physics and the Standard Model

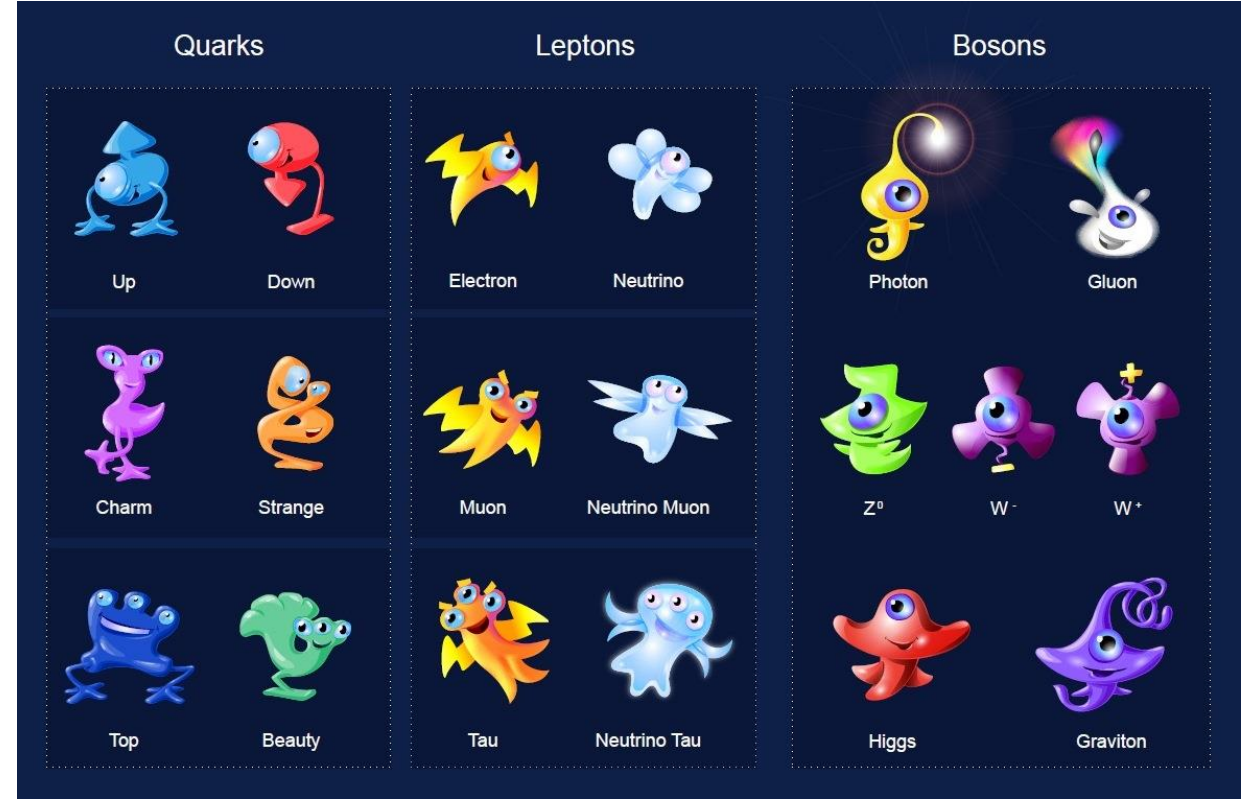
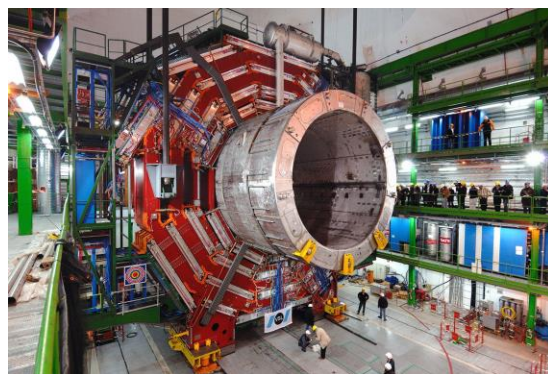


Image sources: CERN

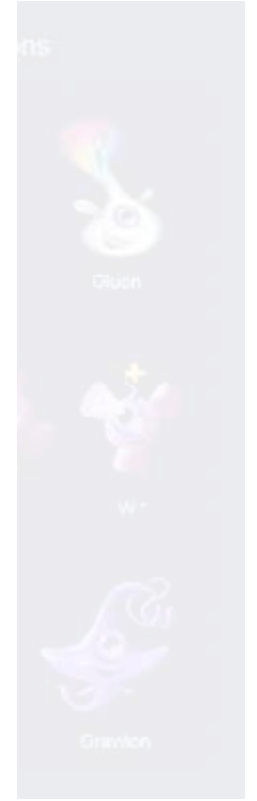
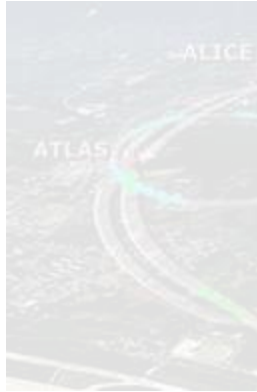
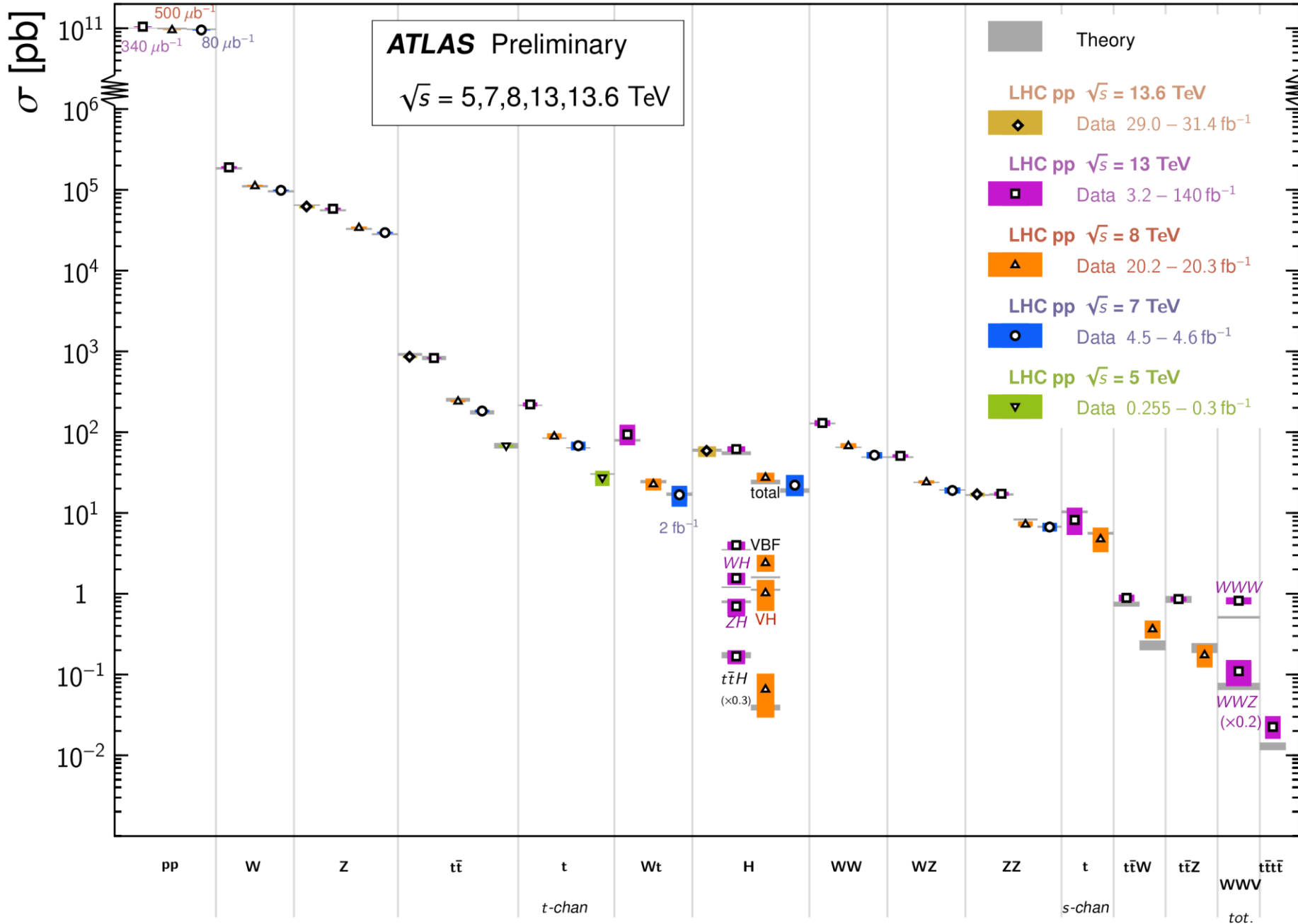
Image source: CERN / ParticleQuest / André-Pierre Olivier



Standard Model Total Production Cross Section Measurements

Status: October 2023

Wt
Part



Why perturbative QCD? (2)

Lattice QCD

$$\sum_n \langle n | e^{-H(T-t)} \mathcal{O} e^{-Ht} | n \rangle = \int d[U_\mu(n)] e^{-\mathcal{A}[U]} \det(D+m) \mathcal{O}[U](t)$$

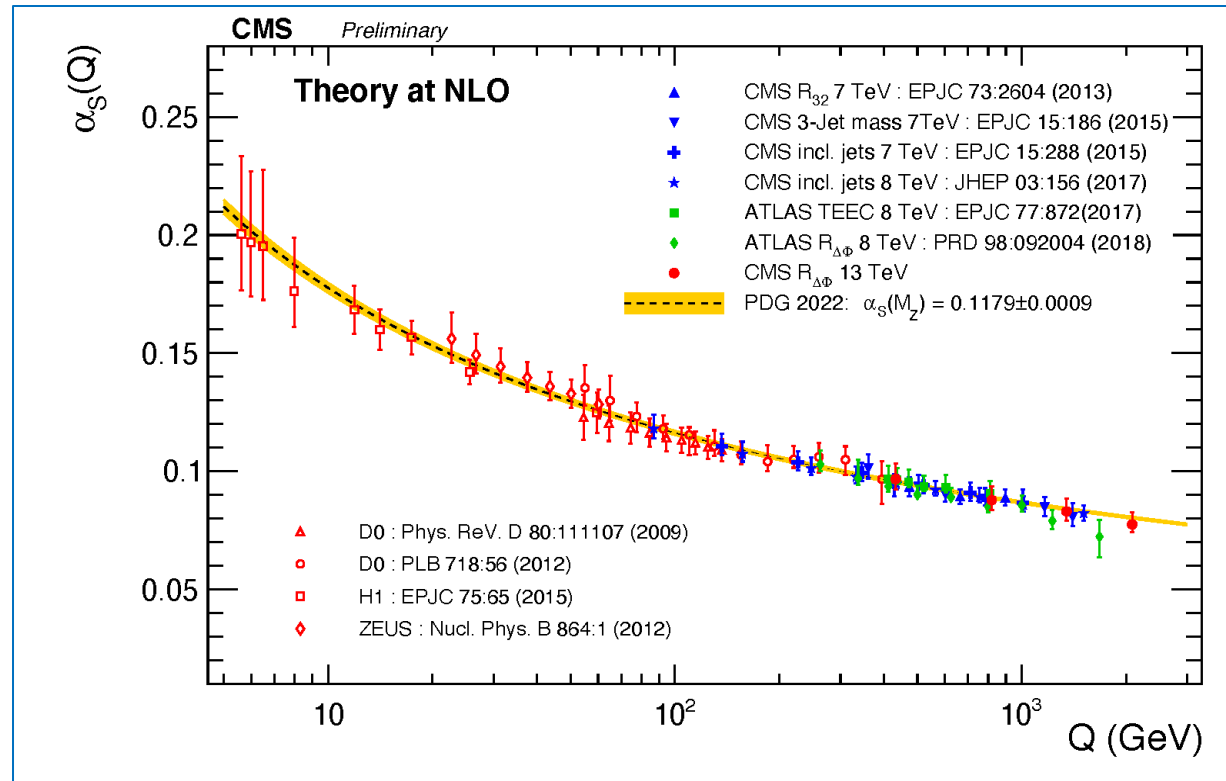
- Very large computational challenge:
 - For a $96^3 \times 192$ lattice: Integrate over five billion variables
 - Integrand contains the determinant of (100 Billion) x (100 Billion) matrix
- Fast code running on 2048 nodes of Frontier sustains 16 Petaflops [10^{15} (adds + mults)/sec]
- Soon to be overtaken by Intel Aurora machine at Argonne

Frontier – ORNL



ACAT 2024 - 3/14/2024 (5)

Slide from Norman Christ's talk yesterday (my highlighting)



Why perturbative QCD (3)

- Very rapid increase in difficulty with each order in α_s
 - Each new order typically takes 10-20 years
 - But vital for producing precise theoretical predictions to compare against experimental measurements
- Highly challenging and computationally intense
 - e.g. multi-loop amplitude calculations
 - e.g. Monte-Carlo integration of cross sections
 - So new techniques and technologies are always needed



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1. Introduction

- Why perturbative QCD?
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- Why now?
- Proposed applications of quantum computing in high-energy physics

2. Background

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- Overview
- Details

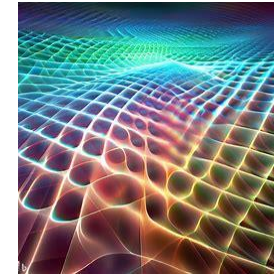
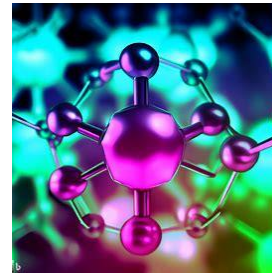
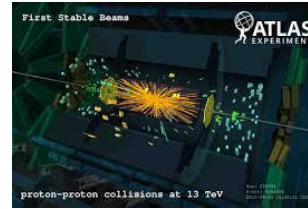
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What can quantum computers do?

- Prime factorisation
- Unstructured search
 - e.g. searching abstract spaces
 - e.g. Monte-Carlo integration
- Simulating quantum systems
 - Computational chemistry
 - Condensed matter systems
 - Lattice QFT/QCD
- Machine learning



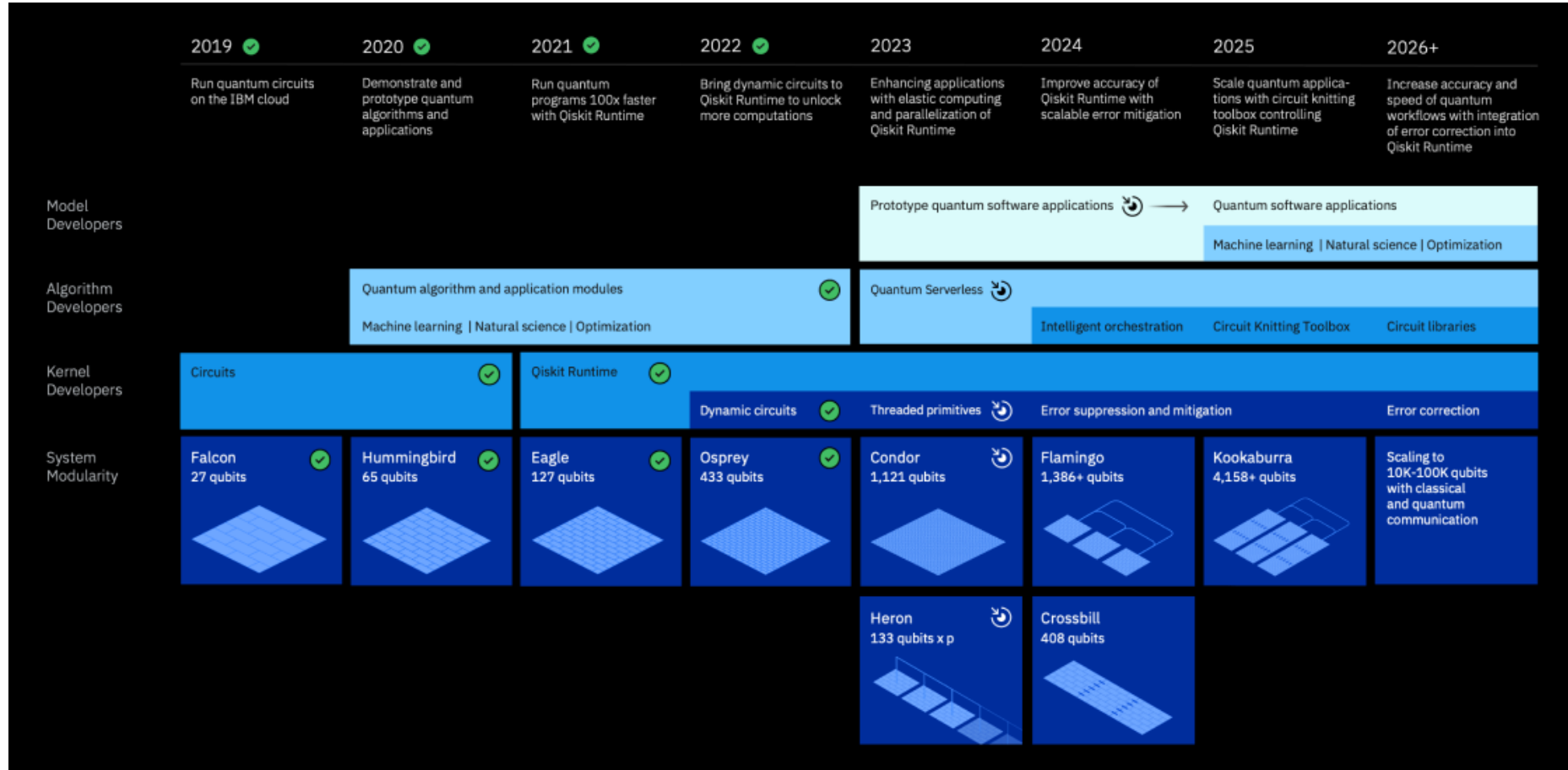
Why now?

- Hardware progress
 - Trapped ions
 - Neutral atoms
 - Photonic systems
 - Superconducting systems
 - ...
- Software progress
 - e.g. Error-correcting codes (e.g. "surface codes")
- Commercial interest



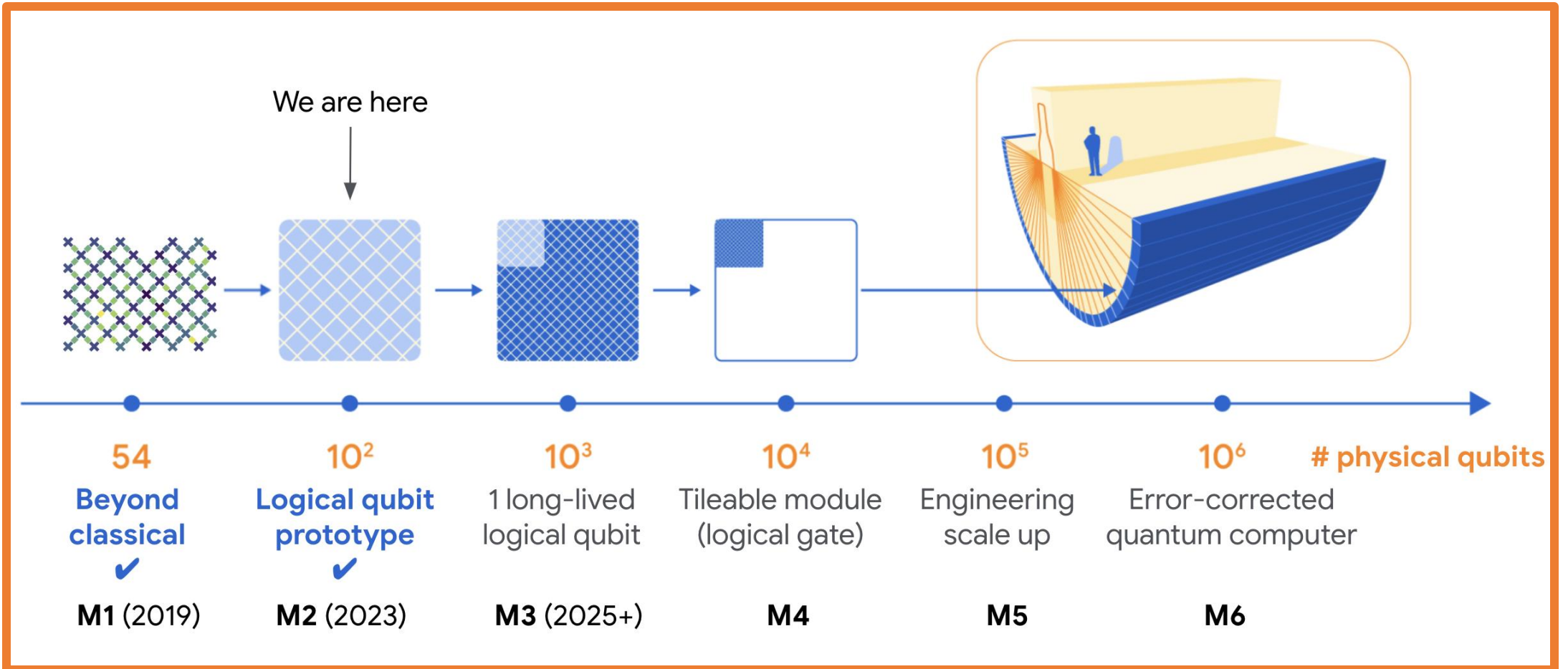
Why now?

IBM Quantum Development Roadmap



Why now?

Google's quantum roadmap



Proposed applications in high-energy physics

- Experiments / data analysis
- PDFs [Pérez-Salinas, Cruz-Martinez, Alhajri, Carrazza, '20], [QuNu Collaboration, '21]
- EFTs [Bauer, Freytsis, Nachman, '21]
- Monte Carlo for cross-sections [Agliardi, Grossi, Pellen, Prati, '22]
- Parton showers [Bauer, de Jong, Nachman, Provasoli, '19], [Bepari, Malik, Spannowsky, Williams, '20], [Gustafson, Prestel, Spannowsky, Williams, '22]
- Event generation [Gustafson, Prestel, Spannowsky, Williams, '22], [Bravo-Prieto, Baglio, Cè, Francis, Grabowska, Carrazza, '21], [Kiss, Grossi, Kajomovitz, Vallecorsa, '22]
- Lattice QCD (See reviews [Klco, Roggero, Savage, '21] and [Bauer et al., '22] and references therein)
- More [Cervera-Lierta, Latorre, Rojo, Rottoli, '17], [Ramírez-Uribe, Rentería-Olivo, Rodrigo, Sborlini, Vale Silva, '21], [Fedida, Serafini, '22], [Clemente, Crippa, Jansen, Ramírez-Uribe, Rentería-Olivo, Rodrigo, Sborlini, Vale Silva, '22]
- 



Spotlight: quantum simulation

- Quantum simulation: a flagship application of quantum computers
- Recent years: proposals for quantum simulation of lattice QFTs (e.g. lattice QCD)
- Quantum simulation of perturbative QCD remains largely unexplored
 - Notable exception: several papers on parton showers
- This talk: first steps towards generic perturbative QCD processes
 - Quantum simulation of **colour** in perturbative QCD
 - Simulation of (more challenging) **kinematics** left to future work



Motivation for quantum simulation of pQCD

1. Perturbative QCD requires quantum-coherent combination of contributions from many unobservable intermediate states
 - natural candidate to exploit superpositions of quantum states in quantum computers
2. Processes with high-multiplicity final states, with full interference effects
3. Improve speed/precision of perturbative QCD predictions by exploiting speed-ups of known quantum algorithms
 - e.g. quantum amplitude estimation; quantum Monte Carlo

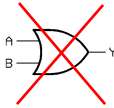


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Quantum circuit model

- Qubits
- Gates
 - Unitary, reversable 
 - Can be controlled by other qubits

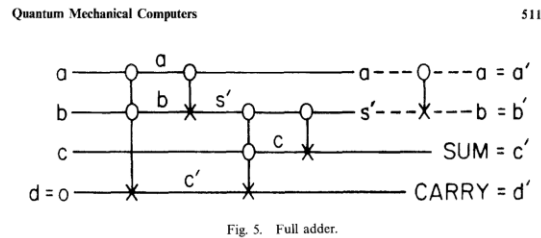
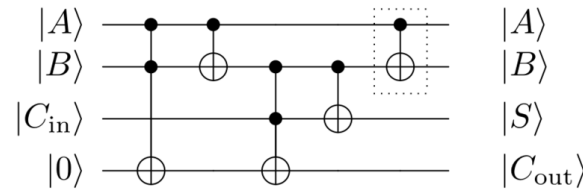






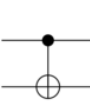
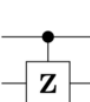
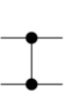

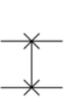
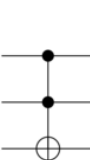


Figure from: Feynman, R.P. Quantum mechanical computers. *Found Phys* 16, 507–531 (1986)

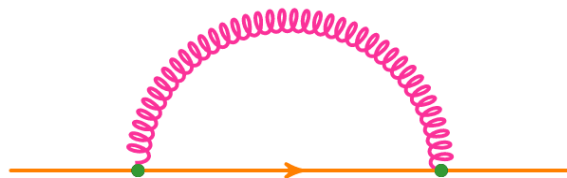


Operator	Gate(s)		Matrix
Pauli-X (X)		\oplus	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)			$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)			$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)			$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)			$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)			$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$



Crash course: colour in QCD calculations

- SU(3) structure function f^{abc} at each triple-gluon vertex
 - (4-gluon vertex can be written as linear combination of 3-gluon vertices)
- SU(3) generator T^a_{ij} at each quark-gluon vertex
- Trace over unmeasured (unmeasurable) colours
- e.g.



$$\sum_{\substack{a \in \{1, \dots, 8\} \\ j \in \{1, 2, 3\}}} T^a_{ij} T^a_{jk}$$

- Note: the large- N_c expansion is not used in this work



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Idea: can Gell-Mann matrices become gates?

$$T_{ij}^a = \frac{1}{2} \lambda_{ij}^a$$

$$\lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda^4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda^6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

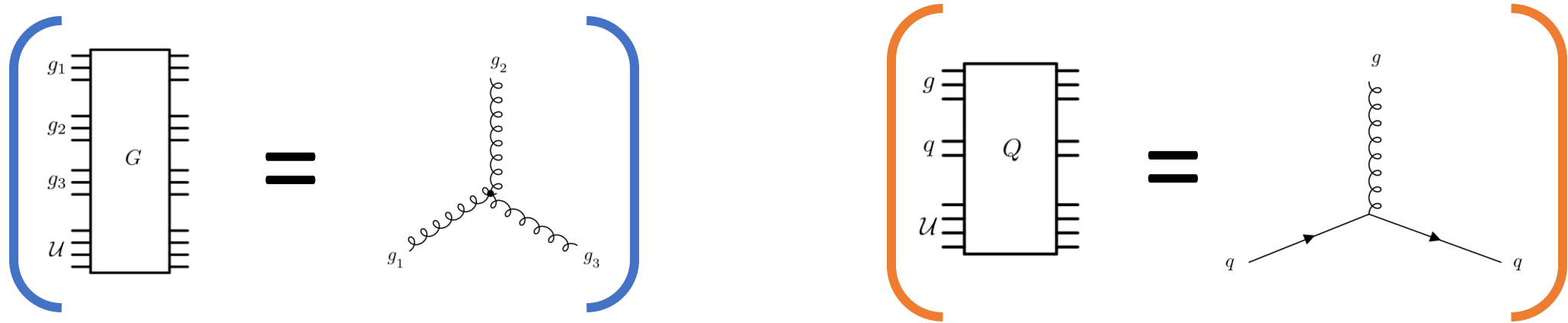
$$\lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

- Short answer: yes, but there are complications:
 - Not $2^n \times 2^n$
 - Not unitary



Key results of this work

- Two quantum gates (**G** and **Q**) to simulate colour parts of the interactions of quarks and gluons

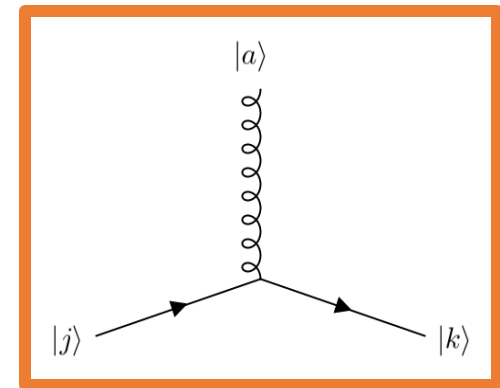


- Explicit construction of these gates: see later

Methods

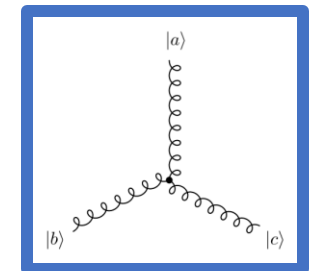
- Quark colours: represented by 2 qubits ($2^2 = 4$ basis states, of which 1 is unused)
- Gluon colours: represented by 3 qubits ($2^3 = 8$ basis states)
- **Quark-gluon interaction gate** is designed such that

$$Q |a\rangle_g |k\rangle_q |\Omega\rangle_{\mathcal{U}} = \sum_{j=1}^3 T_{jk}^a |a\rangle_g |j\rangle_q |\Omega\rangle_{\mathcal{U}} + (\text{terms orthogonal to } |\Omega\rangle_{\mathcal{U}})$$



- **Triple-gluon interaction gate** is designed such that

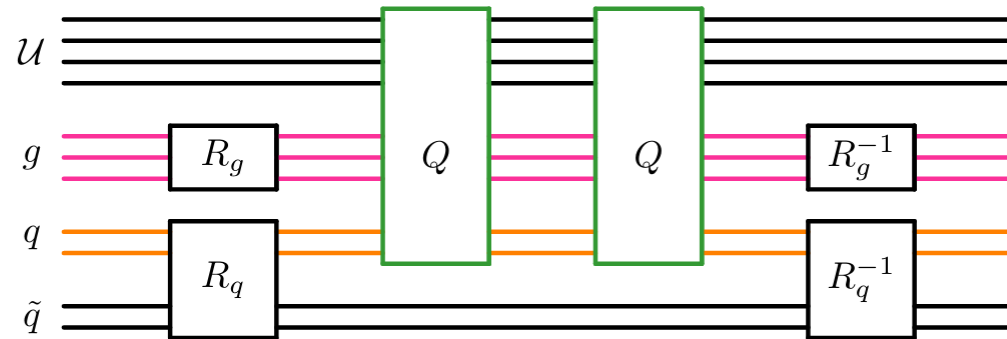
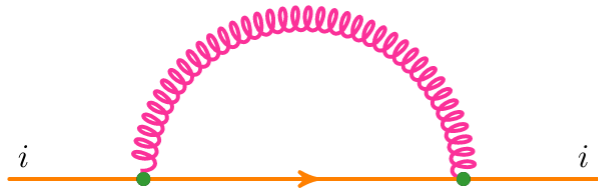
$$G |a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3} |\Omega\rangle_{\mathcal{U}} = f^{abc} |a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3} |\Omega\rangle_{\mathcal{U}} + (\text{terms orthogonal to } |\Omega\rangle_{\mathcal{U}})$$



- Note: $|\Omega\rangle_{\mathcal{U}}$ is a reference state of a "Unitarisation register", which we introduce because in $SU(3)$, T_{jk}^a and f^{abc} are non-unitary.

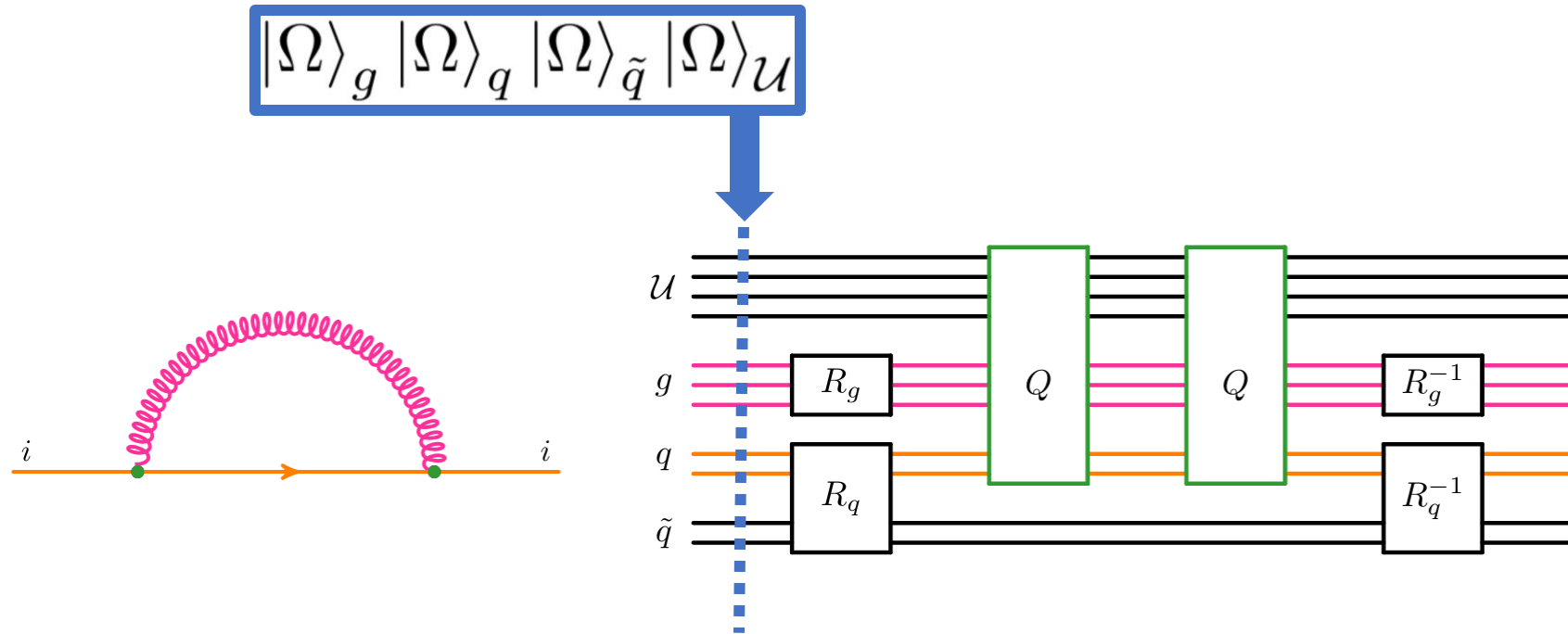
Calculating colour factors: illustrative example

(See later slides for more complicated examples)



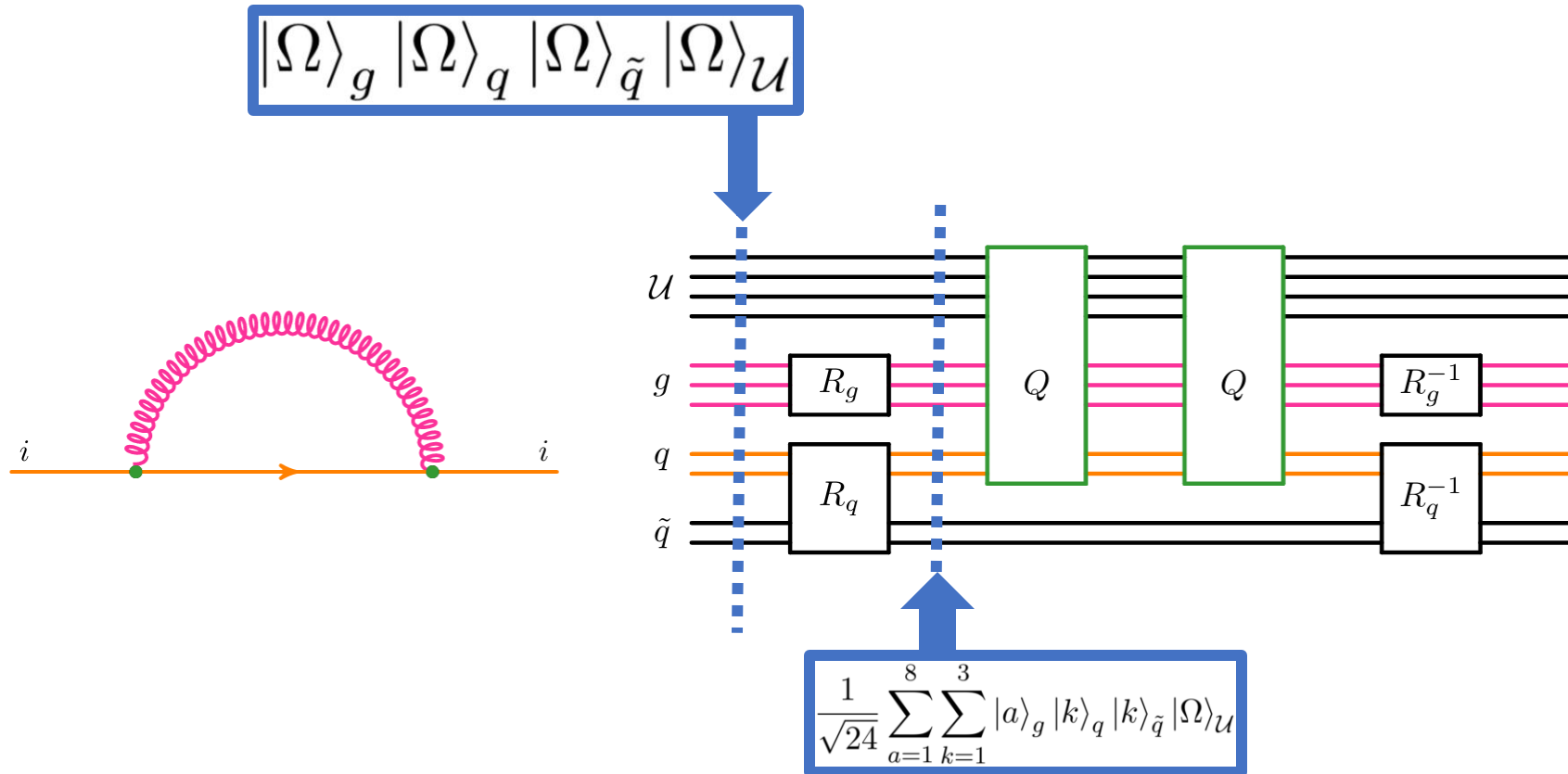
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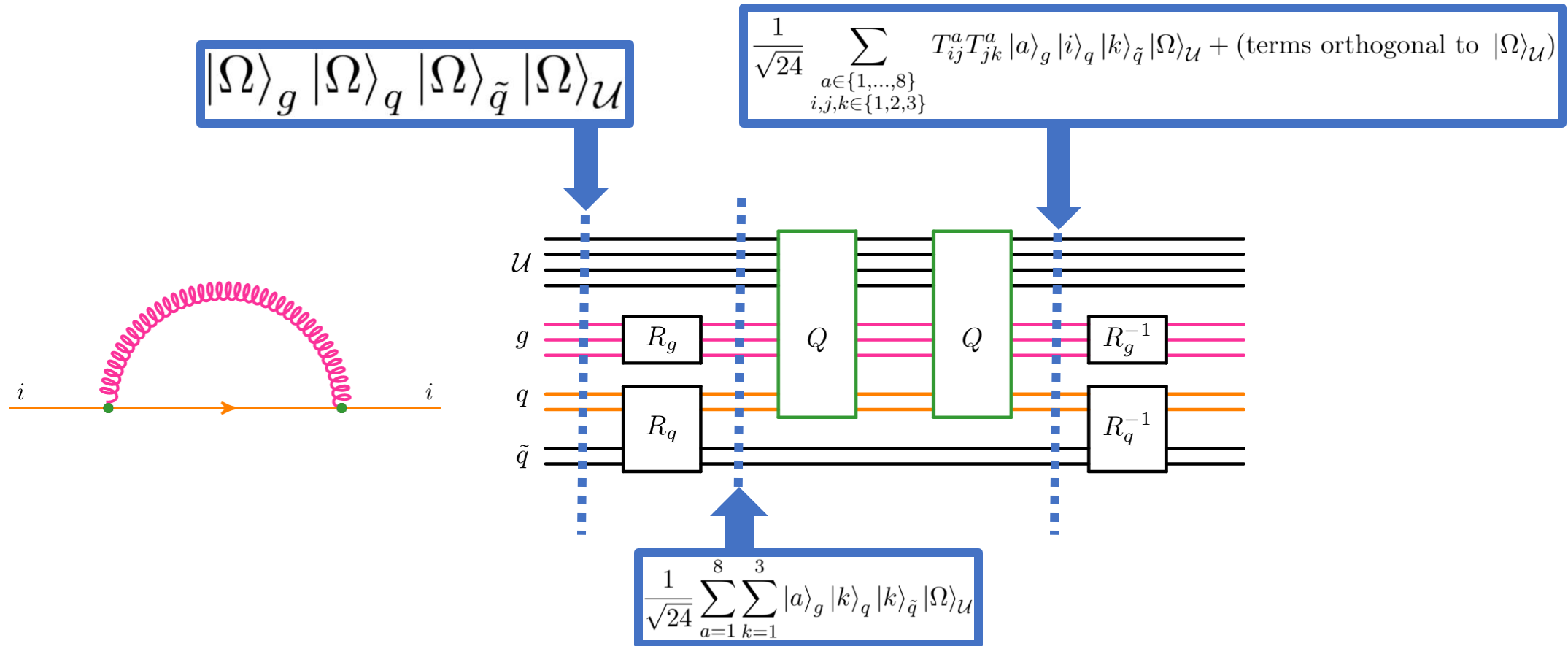


Calculating colour factors: illustrative example

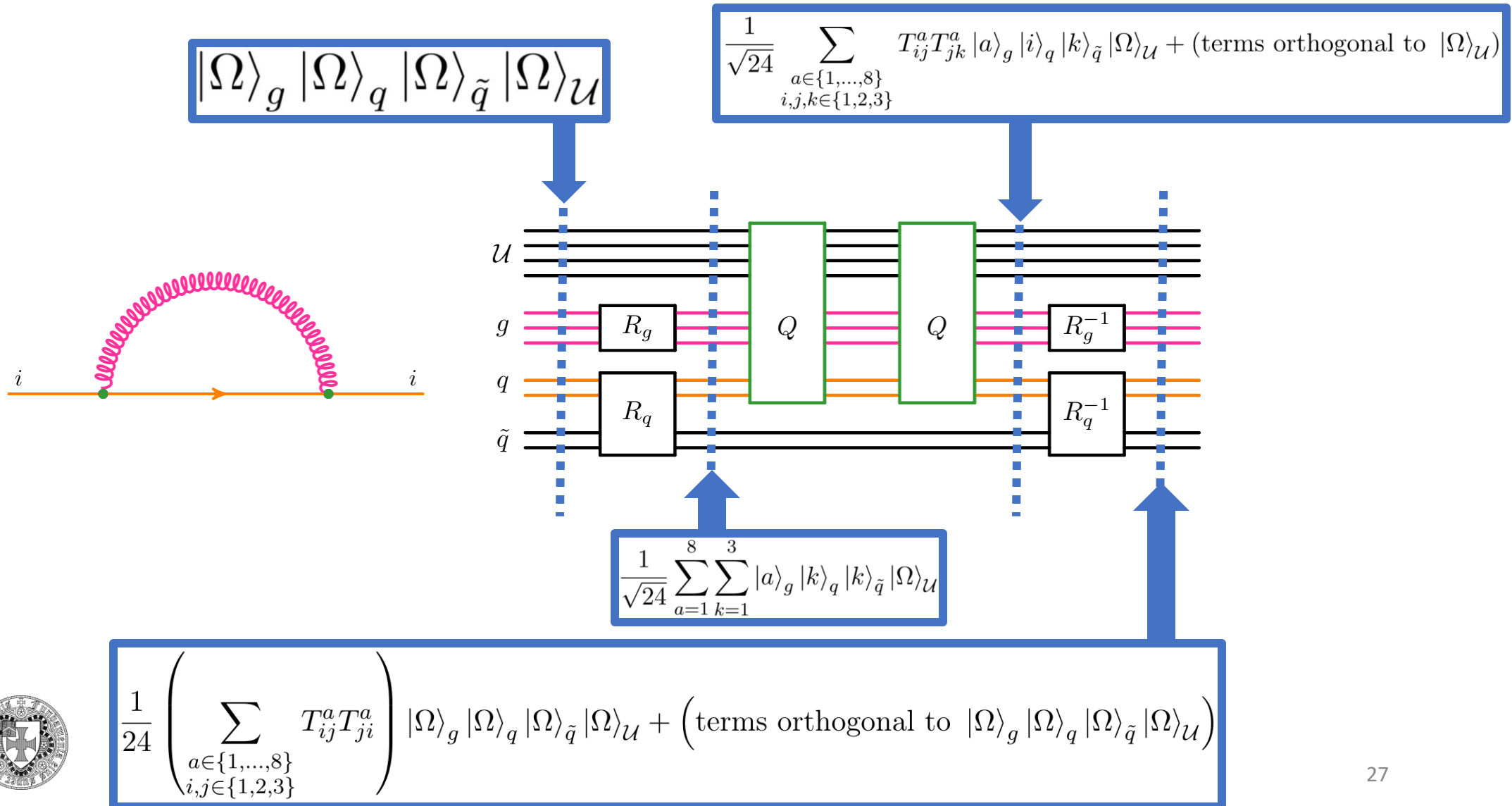
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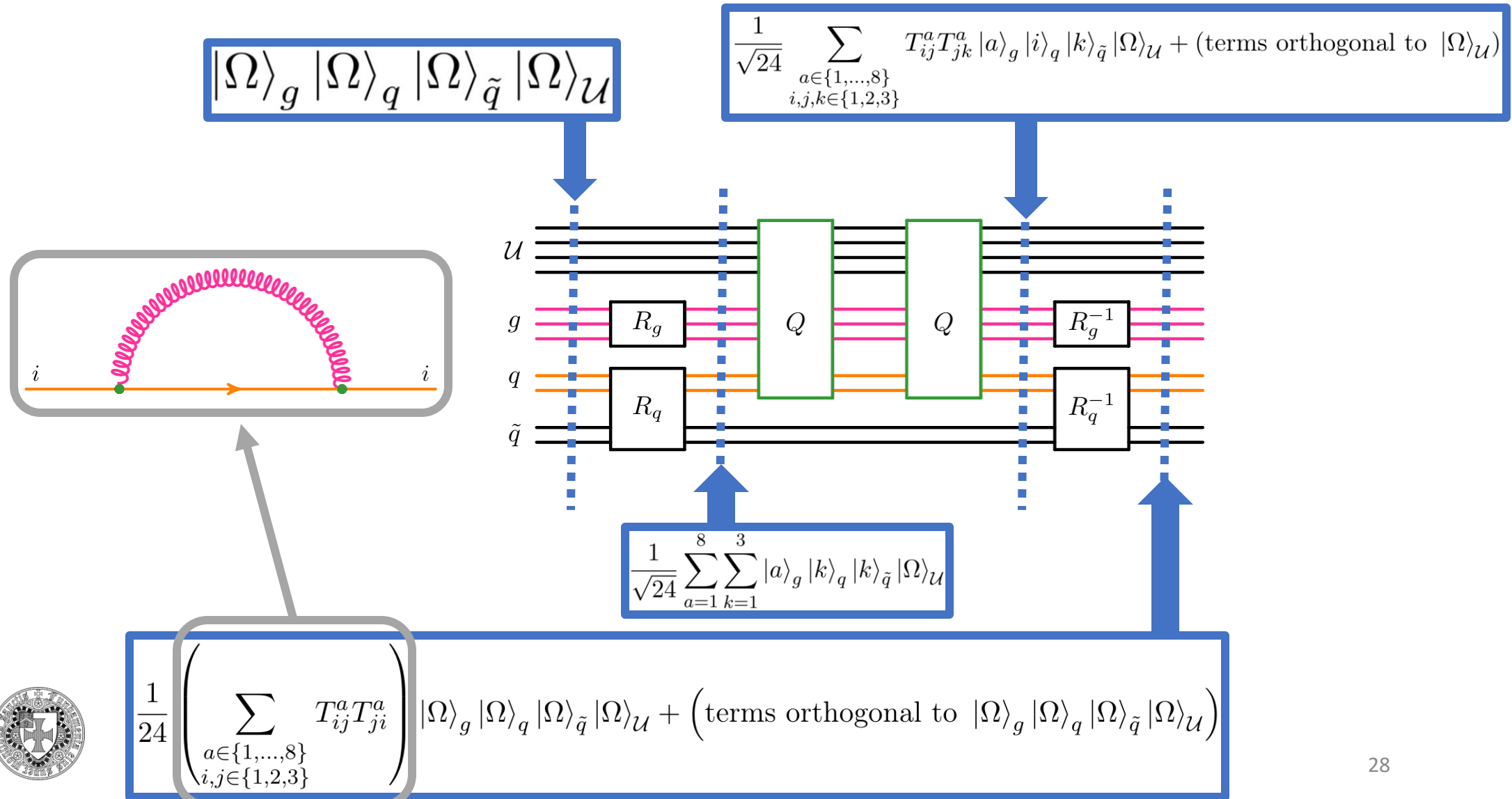
Calculating colour factors: illustrative example



Calculating colour factors: illustrative example



Calculating colour factors: illustrative example

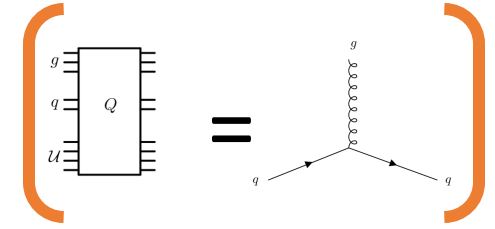


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 - Constructing the Q and G gates
 - General algorithm for calculating colour factors for arbitrary Feynman diagrams
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Construction of the Q gate



$$Q |a\rangle_g |k\rangle_q |\Omega\rangle_U = \sum_{j=1}^3 T_{jk}^a |a\rangle_g |j\rangle_q |\Omega\rangle_U + (\text{terms orthogonal to } |\Omega\rangle_U)$$

- Start by defining matrices $\bar{\lambda}_a$

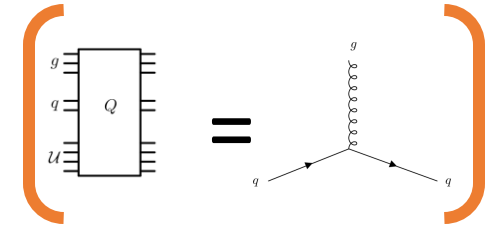
$$\bar{\lambda}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \bar{\lambda}_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \bar{\lambda}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\bar{\lambda}_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \bar{\lambda}_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \bar{\lambda}_6 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\bar{\lambda}_7 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \bar{\lambda}_8 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

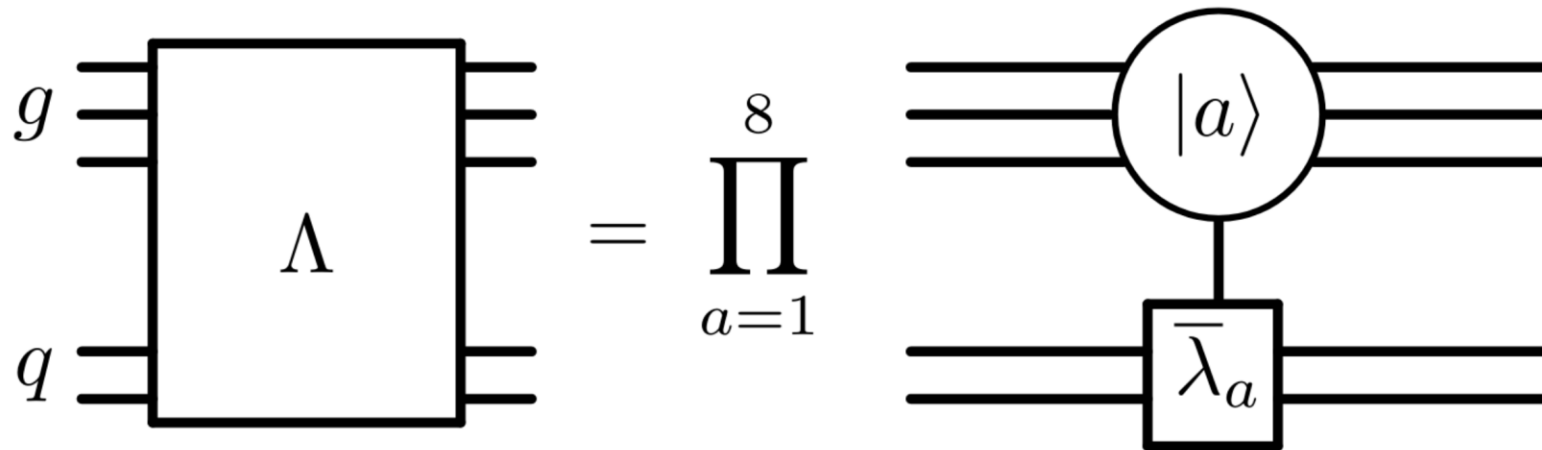


Construction of the Q gate

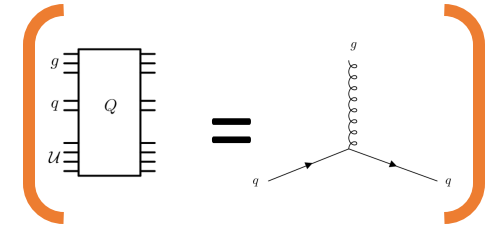


$$Q |a\rangle_g |k\rangle_q |\Omega\rangle_U = \sum_{j=1}^3 T_{jk}^a |a\rangle_g |j\rangle_q |\Omega\rangle_U + (\text{terms orthogonal to } |\Omega\rangle_U)$$

- Next, define a gate Λ

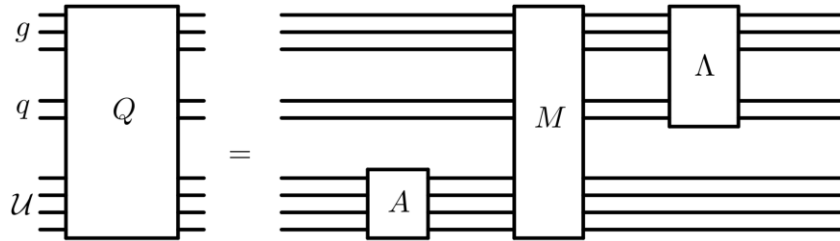


Construction of the Q gate



$$Q |a\rangle_g |k\rangle_q |\Omega\rangle_U = \sum_{j=1}^3 T_{jk}^a |a\rangle_g |j\rangle_q |\Omega\rangle_U + (\text{terms orthogonal to } |\Omega\rangle_U)$$

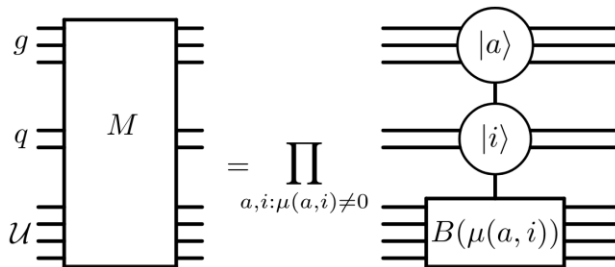
- Finally, define the gate Q



Recall:

$$\langle \Omega | U B(\alpha) A | \Omega \rangle_U = \alpha$$

with



Explicitly:

$$\mu(a, i) = \begin{cases} \frac{1}{2} & \text{if } (\bar{\lambda}_a)_{ij} - (\lambda_a)_{ij} = 0 \quad \forall j \\ \frac{1}{2\sqrt{3}} & \text{if } a = 8 \text{ and } i \in \{1, 2\} \\ \frac{-1}{\sqrt{3}} & \text{if } a = 8 \text{ and } i = 3 \\ 0 & \text{otherwise.} \end{cases}$$

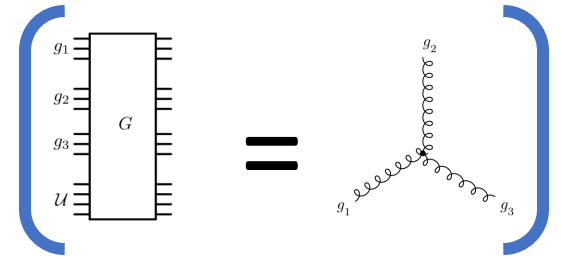
where μ is defined such that $\mu(a, i) \bar{\lambda}_a |i\rangle = \frac{1}{2} \lambda_a |i\rangle$

Recall:

$$\begin{aligned} \bar{\lambda}_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & \bar{\lambda}_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & \bar{\lambda}_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ \bar{\lambda}_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & \bar{\lambda}_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 0 \end{pmatrix}, & \bar{\lambda}_6 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \bar{\lambda}_7 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, & \bar{\lambda}_8 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned}$$

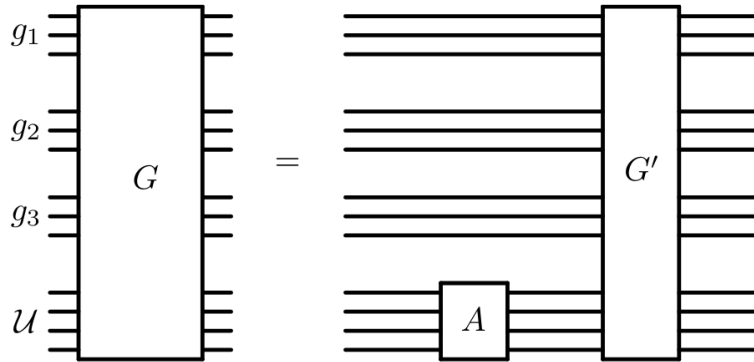


Construction of the G gate



$$G |a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3} |\Omega\rangle_{\mathcal{U}} = f^{abc} |a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3} |\Omega\rangle_{\mathcal{U}} + (\text{terms orthogonal to } |\Omega\rangle_{\mathcal{U}})$$

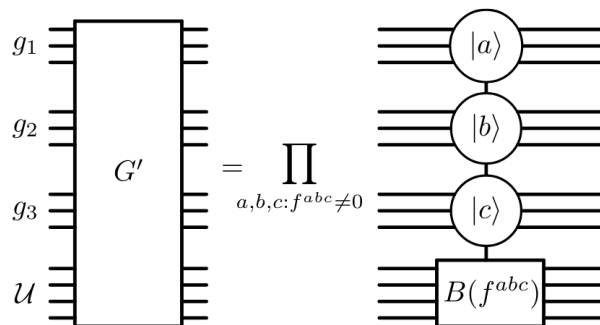
- Define G gate:



Recall:

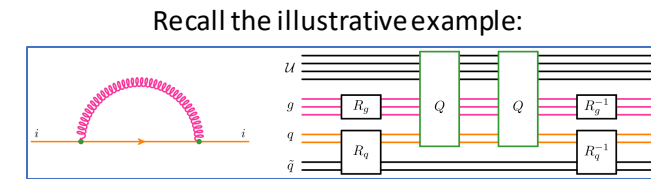
$$\langle \Omega |_{\mathcal{U}} B(\alpha) A | \Omega \rangle_{\mathcal{U}} = \alpha$$

where:



Calculating the colour factor of arbitrary Feynman diagrams

- Build a quantum circuit with:
 - For each gluon, 1 gluon register, with 3 qubits per register
 - For each quark line, a pair of quark registers: q and \tilde{q} , with 2 qubits per register
 - A unitarisation register with $N_U = \lceil \log_2(N_V + 1) \rceil$ qubits
- Initialise each register \mathcal{r} into the state $|\Omega\rangle_{\mathcal{r}}$
- For each gluon, apply R_g
- For each quark, apply R_q
- For each quark-gluon vertex, apply Q gate to the corresponding g and q registers (not \tilde{q})
- For each triple-gluon vertex, apply G gate to the corresponding g registers
- For each gluon, apply $(R_g)^{-1}$
- For each quark, apply $(R_q)^{-1}$
- Colour factor \mathcal{C} is found encoded in the final state of the quantum computer, which is:



$$\frac{1}{\mathcal{N}} \mathcal{C} |\Omega\rangle_{all} + (\text{terms orthogonal to } |\Omega\rangle_{all})$$

$$\text{where } \mathcal{N} = N_c^{n_q} (N_c^2 - 1)^{n_g}$$



Outline

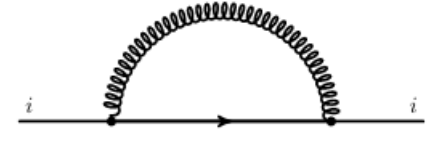
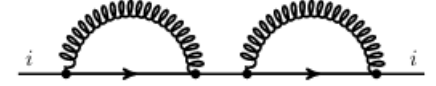
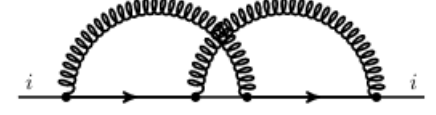

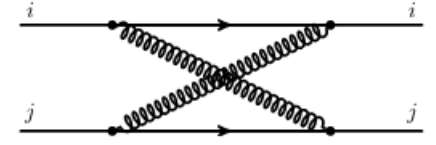
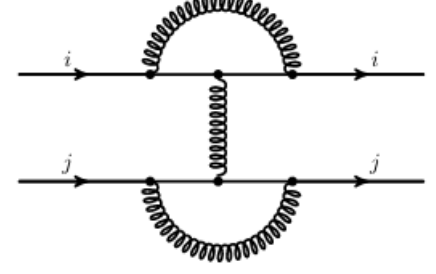
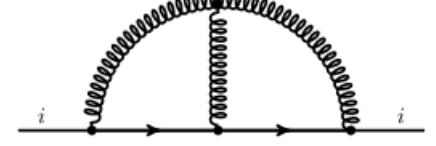
1. Introduction
2. Background
3. Quantum circuits for colour
 - Overview
 - Details
4. **Results/validation**
5. Outlook and summary



Validation

- Implemented using Qiskit (IBM)
- Simulated various diagrams
 - Simulated noiseless quantum computer
 - These examples use up to 30 qubits
 - Ran each diagram 10^8 times
 - Measured output to infer colour factor

$$\frac{1}{\mathcal{N}} \mathcal{C} |\Omega\rangle_{all} + (\text{terms orthogonal to } |\Omega\rangle_{all})$$
 - Full agreement with analytic expectation
- Follow-up work (in progress)
 - Improved algorithm (quadratically faster)
 - Enables interferences of multiple diagrams

Diagram	Analytical	Numerical
	$C_F N = 4$	3.9988 ± 0.0012
	$C_F^2 N = \frac{16}{3}$	5.331 ± 0.010
	$\frac{C_F}{2} = \frac{2}{3}$	0.673 ± 0.010
	$N(N^2 - 1) = 24$	23.95 ± 0.03
	$\frac{(N^2 - 1)}{4} = 2$	2.00 ± 0.03
	0	$0.0^{+0.5}_{-0.0}$
	$\frac{C_F N^2}{2} = 6$	5.92 ± 0.08

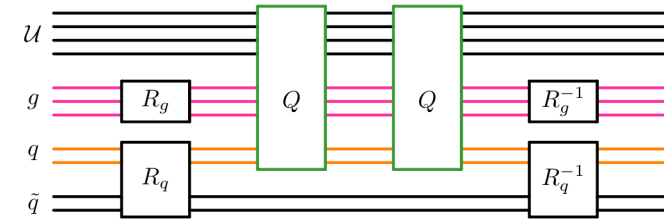
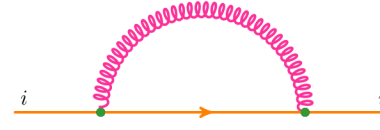


Directions for future work

- Interference of multiple diagrams (work in progress)
 - Natural application for a quantum computer
 - Can try with/without quantum simulation of kinematic parts
- Kinematic parts
 - Unitarisation register could be useful here too
 - Much larger Hilbert space since kinematic variables are continuous
- High-multiplicity processes
- Monte-Carlo integration of cross-sections
 - quadratic speed-up



Summary and outlook



- Designed quantum circuits to simulate colour part of perturbative QCD
 - Example application: colour factors for arbitrary Feynman diagrams
 - First step towards a full quantum simulation of generic perturbative QCD processes
- Natural avenues for follow-up work:
 - Interference of multiple Feynman diagrams (work now in progress)
 - Kinematic parts of Feynman diagrams
 - Use in a quantum-accelerated Monte Carlo calculation of cross-sections
 - Quadratic speed-up over classical Monte Carlo

Backup slides



What quantum computers can and cannot do

- Formally, anything that can be computed on a quantum computer can also be computed on a classical Turing machine

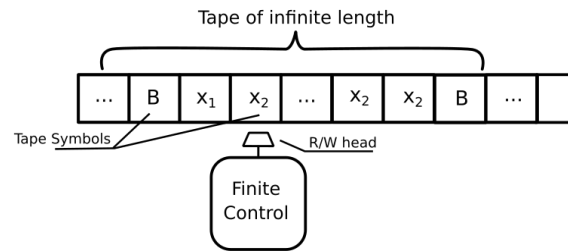


Figure from: [openstax.org](https://openstax.org/r/enggenus)

- But quantum computers are potentially (much) faster than classical computers for certain problems

Example: the increment circuit

$$|k\rangle \rightarrow |k + 1 \pmod{2^N}\rangle$$

- Examples:

- $|00000\rangle \rightarrow |00001\rangle$
- $|01011\rangle \rightarrow |01100\rangle$
- $|11111\rangle \rightarrow |00000\rangle$ (overflow)
- $\frac{\alpha|00000\rangle + \beta|01011\rangle}{|\alpha|^2 + |\beta|^2} \rightarrow \frac{\alpha|00001\rangle + \beta|01100\rangle}{|\alpha|^2 + |\beta|^2}$

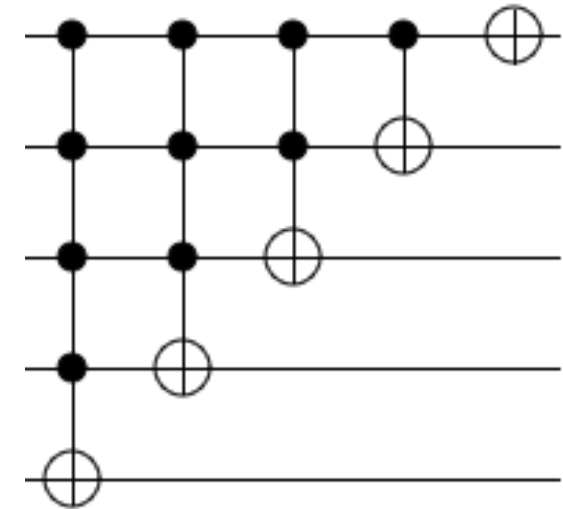


Figure adapted from: algassert.com/circuits/2015/06/12/Constructing-Large-Increment-Gates.html



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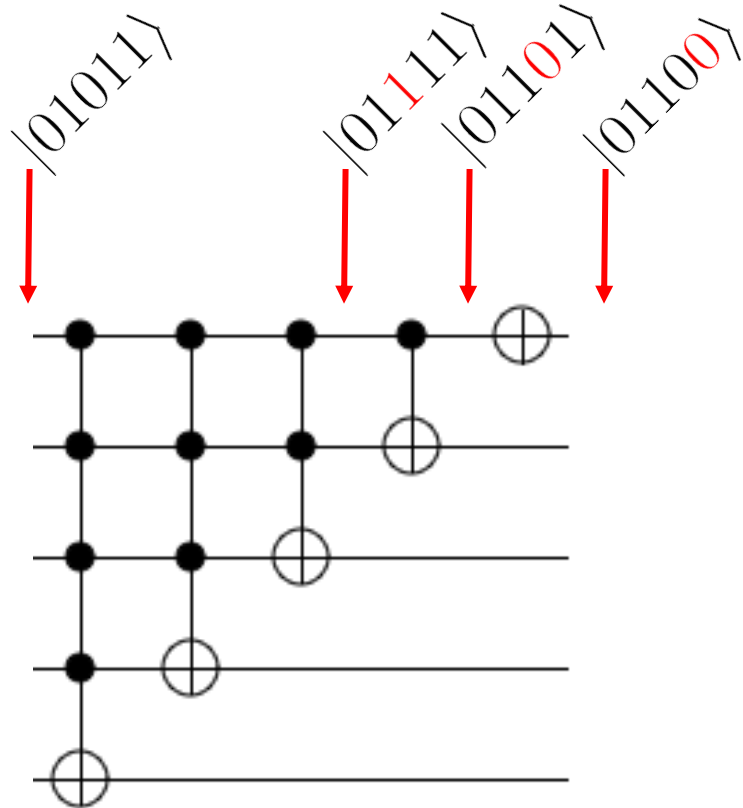


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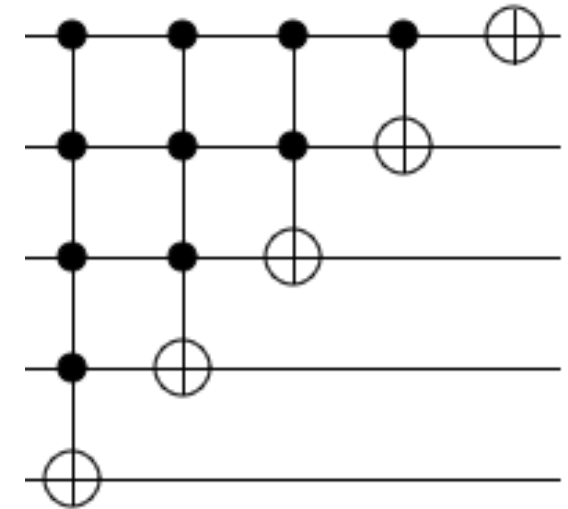


Figure adapted from: algassert.com/circuits/2015/06/12/Constructing-Large-Increment-Gates.html



Non-unitary operators in perturbative QCD

- Would like quantum gates for the 8 linear operators

$$|j\rangle_q \rightarrow \sum_i T_{ij}^a |i\rangle_q$$

and also for the (diagonal) operator

$$|a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3} \rightarrow f^{abc} |a\rangle_{g_1} |b\rangle_{g_2} |c\rangle_{g_3}$$

- An operator is unitary iff the rows of its matrix representation are orthonormal

- In matrices T_{ij}^a and f^{abc} , rows are orthogonal
 - But not necessarily of unit norm

- Need a unitary way to alter a state's norm

Recall:

$$\lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda^4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda^6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$



Unitarisation register: expanding the space

- Let L be an operator acting on a Hilbert space \mathcal{H}_1
- If L is non-unitary, it cannot be directly implemented as a circuit
- But it may be possible to define a new unitary operator \hat{L} acting on a larger space $\mathcal{H}_1 \otimes \mathcal{H}_U$ such that

$$\langle \Omega |_{\mathcal{U}} \langle \chi_2 | \hat{L} | \chi_1 \rangle | \Omega \rangle_{\mathcal{U}} = \langle \chi_2 | L | \chi_1 \rangle$$

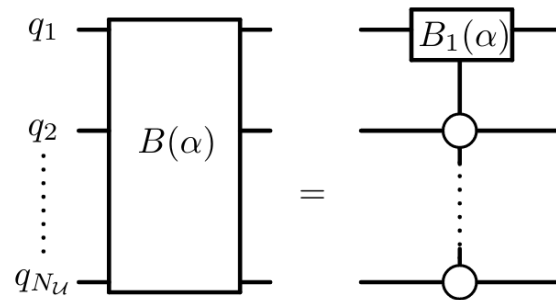
for some state $|\Omega_{\mathcal{U}}\rangle \in \mathcal{H}_U$
for all states $|\chi_1\rangle, |\chi_2\rangle \in \mathcal{H}_1$

- In this work, we introduce a single additional register \mathcal{U} , whose size is small: $N_{\mathcal{U}} = \lceil \log_2(N_V + 1) \rceil$



Unitarisation register: gates A and B

- Let A denote the increment circuit described earlier
- Define a gate $B(\alpha)$:



where:

$$B_1(\alpha) = \begin{pmatrix} \sqrt{1 - |\alpha|^2} & \alpha \\ -\alpha & \sqrt{1 - |\alpha|^2} \end{pmatrix}$$



Unitarisation register: key properties

- Together, gates A and $B(\alpha)$ act on \mathcal{U} in the following way:

$$B(\alpha)A|k\rangle = \begin{cases} \alpha|0\rangle + \sqrt{1-|\alpha|^2}|1\rangle & \text{if } k = 0 \\ |k+1\rangle & \text{if } 0 < k < 2^{N_{\mathcal{U}}} - 1 \\ \sqrt{1-|\alpha|^2}|0\rangle - \alpha|1\rangle & \text{if } k = 2^{N_{\mathcal{U}}} - 1. \end{cases} \quad |0\rangle_{\mathcal{U}} \equiv |\Omega\rangle_{\mathcal{U}}$$

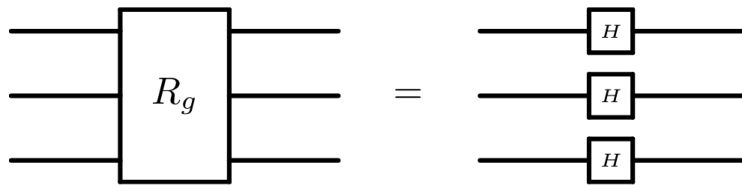
which means we can apply $B(\alpha)A$ repeatedly up to $2^{N_{\mathcal{U}}} - 1$ times and satisfy

$$\langle \Omega |_{\mathcal{U}} \prod_{i=1} \{B(\alpha_i)A\} | \Omega \rangle_{\mathcal{U}} = \prod_{i=1} \alpha_i$$



R_g and R_q gates for tracing

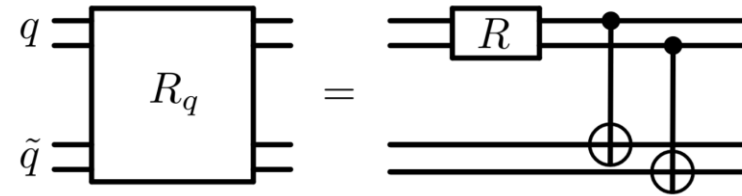
$$R_g |\Omega\rangle_g = \sum_{a=1}^8 \frac{1}{\sqrt{8}} |a\rangle_g$$



$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$R_g^{-1} \sum_{a=1}^8 c_a |a\rangle_g = \left(\frac{1}{\sqrt{8}} \sum_{a=1}^8 c_a \right) |\Omega\rangle_g + (\text{terms orthogonal to } |\Omega\rangle_g)$$

$$R_q |\Omega\rangle_q |\Omega\rangle_{\tilde{q}} = \sum_{k=1}^3 \frac{1}{\sqrt{3}} |k\rangle_q |k\rangle_{\tilde{q}}$$



$$R = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} & 0 \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} & 0 \\ \sqrt{\frac{1}{3}} & 0 & \sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$R_q^{-1} \sum_{i,k \in \{1,2,3\}} c_{ik} |i\rangle_q |k\rangle_{\tilde{q}} = \left(\frac{1}{\sqrt{3}} \sum_{i=1}^3 c_{ii} \right) |\Omega\rangle_q |\Omega\rangle_{\tilde{q}} + (\text{terms orthogonal to } |\Omega\rangle_q |\Omega\rangle_{\tilde{q}})$$

