Quantum computing for High Energy Physics

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Outline

- Intro to quantum computers
- Review of quantum computers in HEP
- Quantum algorithm for helicity amplitudes
- Quantum algorithm for parton showers
- Future outlook for quantum computers
Classical computers have come a long way since 1950s - size of machines (current size of transistor $O(\text{nm})$) and complexity of computers

Quantum computing at a similar stage of development as classical computers in 1950s
7.1. Introducing quantum bits

Let's begin by thinking about a classical bit and a quantum bit.

- **Classical bit**: Can only take on the values 0 and 1. It can be in one of those states and only those. You can look at the bit at any time and, assuming nothing has happened to change the state, it stays in that state.

- **Quantum bit (qubit)**: When we read information from it by a process called measurement, the qubit always becomes the state $|0\rangle$ or $|1\rangle$. However, it is possible to move it to an infinite number of other states and change from one of them to another while we are computing with the qubit before measurement. Measurement says “ok, I’m going to peek at the qubit now” and the result is always a 0 or 1 once you do so. We can then read that out as a bit value of 0 or 1, respectively.

This is weird. This is quantum mechanics and it has amazed, and befuddled, and surprised, and delighted people for close to one hundred years. Quantum computing is based on and takes advantage of this behavior.

Continuing with the right side, we represent all the states the qubit could be in as points on the unit sphere. $|0\rangle$ is at the north pole, and $|1\rangle$ is at the south. Remember: points on the sphere equal quantum states. In the next section I define more precisely what we mean when we write $|0\rangle$ and $|1\rangle$.

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### 2-qubit system

2-qubit system → 4 basis states $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

N qubits → $2^N$ dimensional Hilbert space

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**Power of quantum computing:** this exponential increase in size of Hilbert space
Quantum computing: Two classes/paradigms

**Quantum Annealing**

- Find ground state of Hamiltonian through continuous-time adiabatic process
- Large number of ‘noisy’ qubits
- Good for solving specific problems; for instance optimisation, machine learning.
- D-Wave specialises in quantum annealers

**Quantum Gate Circuit**

- Apply unitary transformations to qubits through discrete set of gates
- Small number of qubits but universal quantum computer
- Google, IBM, Microsoft, Rigetti focused on gate-based quantum computing
Gate-based quantum computers

Classical Computer

Quantum Computer

Gates (classical)
Gates (quantum)

Electrical Signals
Electrical Signals

Measurement Results
Quantum State

INPUT
OUTPUT
Hadamard gate
- One of the most frequently used and important gates in quantum computing
- Has no classical equivalent.
- It puts a qubit initialised in the $|0\rangle$ or $|1\rangle$ state into a superposition of states.

$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$,  
$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$.

Circuit representation

\[
\begin{array}{c}
H \\
\end{array}
\]

Matrix representation

\[
\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}
\]
Quantum gates: CNOT and Toffoli

**CNOT**
- One of the most important gates in QC
- 2-qubit operation that flips the state of a target qubit based on state of a control qubit.
- This is used to create entangled qubits.

\[
\begin{align*}
\text{CNOT}|00\rangle &= |00\rangle, \\
\text{CNOT}|10\rangle &= |11\rangle, \\
\text{CNOT}|01\rangle &= |01\rangle, \\
\text{CNOT}|11\rangle &= |10\rangle.
\end{align*}
\]

**Matrix representation**
\[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{bmatrix}
\]

**Circuit representation**

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**Toffoli (CCNOT)**
- 3-qubit operation, an extension of CNOT gate but on 3 qubits
- Flips the state of a target qubit based on state of the 2 other control qubits

\[
\begin{align*}
\text{CCNOT}|000\rangle &= |000\rangle, \\
\text{CCNOT}|100\rangle &= |100\rangle, \\
\text{CCNOT}|110\rangle &= |111\rangle, \\
\text{CCNOT}|001\rangle &= |001\rangle, \\
\text{CCNOT}|010\rangle &= |010\rangle, \\
\text{CCNOT}|111\rangle &= |110\rangle.
\end{align*}
\]

**Matrix representation**
\[
\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

**Circuit representation**
Quantum supremacy?

*Google claimed quantum supremacy with 54-qubit quantum computer - performed a random sampling calculation in 3 mins, 20 sec.*

*They claimed the this would take 10,000 years to do on classical machine.*

*IBM counterclaim: can be done on classical machine in 2.5 days*
Quantum computing in High Energy Physics
One of the key challenges at HL-LHC: track reconstruction in a very busy, high pileup environment (140 - 200 overlapping pp collisions)

Much more CPU and storage needed

Can quantum computers help?
• Express problem of pattern recognition as that of finding the global minimum of an objective function (QUBO)
• Use D-Wave quantum annealer as minimiser (D-Wave 2X (1152 qubits))
• Use triplets (set of 3 hits); which triplets belong to the trajectory of a charged particle.

Minimise function $O :$ equivalent to finding the ground state of the Hamiltonian

$$O(a, b, T) = \sum_{i=1}^{N} a_i T_i + \sum_{i}^{N} \sum_{j < i}^{N} b_{ij} T_i T_j \quad T_i, T_j \in \{0, 1\}$$

- weights quality of individual triplets based on physics properties
- encodes relationship between triplets

Minimising $O = $ selecting the best triplets to form track candidates.
Track reconstruction at HL-LHC

- Use dataset representative of HL-LHC
- Study performance of algorithm as a function of particle multiplicity
- Similar purity and efficiency as current algorithms
- Execution time of algorithm not expected to scale with track multiplicity

Overall timing still needs to be measured and studied, but physics performance of tracking algorithm similar to classical

https://hep-qpr.lbl.gov
• Precise measurement of Higgs boson properties requires selecting large and high purity sample of signal events over a large background
• Use quantum and classical annealing to solve a Higgs signal over background machine learning optimisation problem
• Map the optimization problem to that of finding the ground state of a corresponding Ising spin model.

Build a set of weak classifiers from kinematic observables of a $H \rightarrow \gamma\gamma$ decay, use these to construct a strong classifier
Map a signal vs background optimization problem to that of finding the ground state of a corresponding Ising spin model.

1098 active qubits

Comparable performance to current state of the art machine learning methods, with some advantage for small training datasets

First application of D-Wave quantum annealing to a scenario in HEP
Quantum algorithm for helicity amplitudes and parton showers

in collaboration with Simon Williams¹, Khadeeja Bepari² and Michael Spannowsky²

¹Imperial College London
²IPPP
Collision event at LHC

*Diagram taken from Pierpaolo Mastrolia lecture*
Collision event at LHC

- Hard interaction + parton shower: can be described perturbatively + independent of non-perturbative processes.
- Most time consuming stages of event generation.
• Scattering amplitudes - **essential** for calculating predictions for collider experiments.

• At LHC, collisions **dominated by QCD processes**, which carry large theoretical uncertainty due to limited knowledge of higher order terms in perturbative QCD

• Improving accuracy of theoretical predictions of cross-sections means computing **loop amplitudes and tree level amplitudes** of higher multiplicities.

• Conventional method of computing an unpolarised cross section involves squaring the amplitude at the beginning and then summing analytically over all possible helicity states using trace techniques

• For complex processes, this approach is not very feasible. For $N$ feynman diagrams for an amplitude, there are $N^2$ terms in the square of the amplitude
Spinor helicity formalism

- Tool for calculating scattering amplitudes much more efficiently than conventional approach. Greatly simplifies the calculation of scattering amplitudes for complex processes.

Compute amplitudes of fixed helicity setup which has the advantage:

- For massless particles, chirality and helicity coincide. Chirality is preserved by gauge interactions, hence helicity is also conserved. Helicity basis an optimal one for massless fermions.

- Different helicity configurations do not interfere. Full amplitude obtained by summing the squares of all possible helicity amplitudes. \( \sum_{\text{helicity}} |M_n|^2 \).

- Using recursion relations such as BCFW, it is possible to calculate multi-gluon scattering amplitudes which would be prohibitive using traditional methods.
Helicity amplitude calculations based on manipulation of helicity spinors

Helicity spinors for massless states can be expressed as:

\[ |p\rangle^\hat{a} = \sqrt{2E} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix} \]

Qubits can be represented on a Bloch sphere as a linear superposition of orthonormal basis states \( |0\rangle \) and \( |1\rangle \) as:

\[ |\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\varphi} \sin \frac{\theta}{2} |1\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix} \]

Spinors naturally live in the same representation space as qubits, thus helicity spinors can be represented as qubits.
Equivalence between spinors and qubits

Calculation of helicity amplitudes follows same structure as a quantum computing algorithm; quantum operators act on an initial state to transform it into a state that can be measured

- Encode operators acting on spinors as a series of unitary transformations in the quantum circuit
- These unitary operations are applied to qubits to calculate helicity amplitude

Visualisation of helicity spinors
1→2 helicity amplitude calculation

A simple application of the helicity amplitude approach is the calculation of a 1→2 process

\[ \mathcal{M}_{gq\bar{q}} = \langle \mathbf{p}_f | \vec{\sigma}_\mu | \mathbf{p}_f^\dagger \rangle \epsilon_\pm^\mu, \]

- Gluon polarisation vectors given by:
  \[ \epsilon_+^\mu = -\frac{\langle q | \vec{\sigma}_\mu | p \rangle}{\sqrt{2} \langle qp \rangle}, \quad \epsilon_-^\mu = -\frac{\langle p | \vec{\sigma}_\mu | q \rangle}{\sqrt{2} \langle qp \rangle}. \]

- Can create circuit where each 4-vector calculated individually on 4 qubits - but this will require many qubits and large circuit depth.

- Instead, simplify amplitude using Fierz identity (hence reduce qubits from 10 → 4)

\[
\begin{align*}
\mathcal{M}_+ &= -\sqrt{2} \frac{\langle p_f q | [p_f \bar{p}] \rangle}{\langle qp \rangle}, & \mathcal{M}_- &= -\sqrt{2} \frac{\langle p_f p \rangle [p_f \bar{q}] \rangle}{\langle qp \rangle}.
\end{align*}
\]
isolating the individual helicity processes on the quantum circuit, and removing the su-
computer's performance does not match that of a perfect machine, as expected. Therefore,
leading to a total of 819,200 shots of the algorithm. Figure run without a noise profile for 10,000 shots. The results agree well with theoretically
of the helicity amplitude, calculated using the S@M software.

As a consequence of this simplification, the number of qubits needed to calculate the am-
operations needed in the algorithm. The Santiago machine is a 5-qubit
The results from the quantum computer, shown in Fig.

With this, the amplitude for the
helicity of the process which has been calculated can be identified from the distinct prob-
angles, with runs on the IBM Q 32-qubit Quantum Simulator.

However, it should be noted that a comparison to a perfect machine may not be a fair
ability distributions, one cannot determine the explicit amplitude from the real machine.

Figure 3 shows the results of the algorithm for a random selection of small scattering
vertex circuit. The amplitude for the process is calculated on the
vertex becomes

\[ \mathcal{M}_+ = -\sqrt{2} \frac{\langle p_f q \rangle [p_\tau p]}{\langle q p \rangle}, \quad \mathcal{M}_- = -\sqrt{2} \frac{\langle p_f p \rangle [p_\tau q]}{[q p]} . \]
1→2 helicity amplitude circuit

\[ M_+ = -\sqrt{2} \frac{\langle pfq \rangle\langle pfp \rangle}{\langle qp \rangle}, \quad M_- = -\sqrt{2} \frac{\langle pfp \rangle\langle pTq \rangle}{\langle qp \rangle}. \]
qubits calculate the 3 scalar products for each helicity amplitude

\[ M_+ = -\sqrt{2} \frac{\langle pfq \rangle [pfp]}{\langle qp \rangle}, \quad M_- = -\sqrt{2} \frac{\langle pfq \rangle [pfp]}{[qp]} . \]

Measure these qubits at end of algorithm

- Helicity register controls the helicity of each particle. Using a Hadamard gate, we introduce a superposition between the helicity states \( |+\rangle = |1\rangle \) and \( |--\rangle = |0\rangle \)

- Hence, calculate the helicity of each particle involved simultaneously!
1→2 helicity amplitude calculation

Run algorithm on:
- IBM Q 32-qubit simulator (10,000 shots) without noise profile
- IBM Q 5-qubit Santiago quantum computer (819,200 shots)
1→2 helicity amplitude calculation

Run algorithm on:
- IBM Q 32-qubit simulator (10,000 shots) without noise profile
- IBM Q 5-qubit Santiago quantum computer (819,200 shots)
1→2 helicity amplitude calculation

Run algorithm on:
- IBM Q 32-qubit simulator (10,000 shots) without noise profile
- IBM Q 5-qubit Santiago quantum computer (819,200 shots)

Qubit mapping for IBM Q Santiago machine

Qubit setup in our algorithm

Optimal qubit setup to reduce CNOT errors and limit the number of SWAP operations
1→2 helicity amplitude calculation

Run algorithm on:
- IBM Q 32-qubit simulator (10,000 shots) without noise profile
- IBM Q 5-qubit Santiago quantum computer (819,200 shots)
- Compare with theoretical calculation

Figure 4: Results for the $q\bar{q}$ vertex, positive helicity. Comparison between theoretically calculated probability distribution, quantum simulator and real quantum computer.

The main source of error in the quantum computer is readout noise. Error mitigation methods have been used to optimise the output from the quantum computer and reduce readout noise effects. This has been done using the Qiskit Ignis software [41], which provides tools for noise characterisation and error correction based on noise models of the quantum machines. The method involves testing simple qubit states on a series of calibration circuits, which are run using the quantum simulator with the noise profile of the Santiago machine. The response matrix created from this is shown in Fig. 5. This response matrix is then applied to the machine results to obtain the error corrected results, as shown in Fig. 4.

The response matrix is calculated immediately before running the algorithm.

- Run algorithm on:
  - IBM Q 32-qubit simulator (10,000 shots) without noise profile
  - IBM Q 5-qubit Santiago quantum computer (819,200 shots)
  - Compare with theoretical calculation

- Positive helicity
- Negative helicity
2→2 helicity amplitude calculation

Extending from the 1 → 2 process, we consider the 2 → 2 scattering case of \( q\bar{q} \rightarrow q\bar{q} \)

Amplitudes for the s and t-channel:

\[
\mathcal{M}_{s(+-+-)} = -\langle 2|\bar{\sigma}\mu|1\rangle \frac{1}{s_{12}} \langle 3|\sigma\mu|4\rangle, \quad \mathcal{M}_{s(+-+-)} = -\langle 2|\bar{\sigma}\mu|1\rangle \frac{1}{s_{12}} \langle 3|\bar{\sigma}\mu|4\rangle
\]

\[
\mathcal{M}_{t(+-+-)} = -\langle 3|\bar{\sigma}\mu|1\rangle \frac{1}{s_{13}} \langle 2|\sigma\mu|4\rangle, \quad \mathcal{M}_{t(+-+-)} = -\langle 3|\bar{\sigma}\mu|1\rangle \frac{1}{s_{13}} \langle 2|\bar{\sigma}\mu|4\rangle
\]

Again using the Fiery identity, can simplify these to (reduce # of qubits needed from 17 to 12) :

\[
\mathcal{M}_{t(+-+-)} = 2\frac{\langle 34|21\rangle}{\langle 13|31\rangle}, \quad \mathcal{M}_{t(+-+-)} = 2\frac{\langle 32|41\rangle}{\langle 13|31\rangle}
\]

\[
\mathcal{M}_{s(+-+-)} = 2\frac{\langle 24|31\rangle}{\langle 12|21\rangle}, \quad \mathcal{M}_{s(+-+-)} = 2\frac{\langle 23|41\rangle}{\langle 12|21\rangle}
\]
Run algorithm on:
- IBM Q 32-qubit simulator (10,000 shots)
- Compare with theoretical calculation

Algorithm calculates the positive and negative helicity of each particle involved AND the s and t-channels simultaneously!
After the hard interaction, the next step in simulating a scattering event at LHC is the parton shower.

Parton shower evolves the scattering process from the hard interaction scale down to the hadronisation scale.

Propose a quantum computing algorithm that simulates collinear emission in a 2-step parton shower.

This algorithm builds on previous work by Bauer et. al. (arXiv:1904.03196).

To comply with capability of quantum computers we had access to, consider a simplified model of the parton shower consisting of only one flavour of quark.
Parton shower

- Collinear emission occurs when a parton splits into two massless particles which have parallel 4-momenta.
- The total momentum, \( P \), of the parton is distributed between the particles as: \( p_i = zP, \quad p_j = (1 - z)P \).
- Emission probabilities are calculated using collinear splitting functions, which at LO are given by:

\[
\begin{align*}
P_{q\rightarrow qg}(z) &= C_F \frac{1 + (1 - z)^2}{z}, \\
P_{g\rightarrow q\bar{q}}(z) &= n_f T_R(z^2 + (1 - z)^2), \\
P_{g\rightarrow gg}(z) &= C_A \left[ 2 \frac{1 - z}{z} + z(1 - z) \right].
\end{align*}
\]

Non-emission probability calculated using Sudakov factors

\[
\Delta_{i,k}(z_1, z_2) = \exp \left[ - \alpha_s^2 \int_{z_1}^{z_2} P_k(z') dz' \right],
\]

Probability of a splitting is given by,

\[
\text{Prob}_{k\rightarrow ij} = (1 - \Delta_k) \times P_{k\rightarrow ij}(z).
\]
Circuit for parton shower algorithm

- Circuit comprises of particle registers, emission registers, and history registers and uses a total of 31 qubits.

![Circuit Diagram]

**Count gate**
Uses series of NOT, CNOT and Toffoli (CCNOT) gates to count number of each type of particle.

**Emission gate**
Implements the Sudakov factors using a rotation, which changes the state of the emission gate to $|1\rangle$ if emission, $|0\rangle$ if not.

**History gate**
Determines which emission has occurred.

Update gate
If there is an emission, changes content of particle counts accordingly.

Reset
For next step.
2-step parton shower: initial state a gluon

- Classical Monte Carlo methods need to manually keep track of individual shower histories, which must be stored on a physical memory device.
- Quantum computing algorithm constructs a wavefunction for the whole process and calculates all possible shower histories simultaneously!
Results for parton shower algorithm

Run 10,000 shots on IBM Q 32-qubit Quantum Simulator

We also present a quantum algorithm for simulating collinear emission in a two-step, discrete parton shower with a maximum of three final state particles, utilising the quantum computer's ability to remain in a quantum state throughout the simulation. In contrast

(a) Initial particle a gluon.
(b) Initial particle a quark.
(c) Initial particle an antiquark.

Figure 9: Results from the quantum circuit compared to theoretical predictions for two steps of the parton shower with momentum interval of $z_{\text{lower}} = 0.3$ to $z_{\text{upper}} = 0.5$ and the initial state particle of (a) gluon, (b) quark and (c) antiquark.

Two step parton shower: $z_{\text{up}} = 0.5$, $z_{\text{low}} = 0.3$ (10000 shots)
Results for parton shower algorithm

We also present a quantum algorithm for simulating collinear emission in a two-step, discrete parton shower with a maximum of three final state particles, utilising the quantum computer's ability to remain in a quantum state throughout the simulation. In contrast – 17 –

Figure 9: Results from the quantum circuit compared to theoretical predictions for two steps of the parton shower with momentum interval of $z_{\text{lower}} = 0.3$ to $z_{\text{upper}} = 0.5$ and the initial state particle of (a) gluon, (b) quark and (c) antiquark.

(b) Initial particle a quark.
Summary of parton shower algorithm

- Algorithm builds on previous work by Bauer et. al. [1] by including a vector boson and boson splittings → significant changes in its implementation

- Can simulate both gluon and quark splittings, thus provides the foundations for developing a general parton shower algorithm

- With advancements in quantum technologies, algorithm can be extended to include all flavours of quarks without adding disproportionate computational complexity

[1]: arXiv:1904.03196
Summary of arXiv:2010.00046

- Modeling complexity of collisions at LHC relies on theoretical calculations of multi-particle final states.

- Working with quantum objects and quantum phenomena; can quantum computers help?

- Propose general and extendable quantum algorithms to calculate the hard interaction using helicity amplitudes and a 2-step parton shower

**Helicity amplitude algorithm** exploits equivalence of spinors and qubits, encodes operators as unitary operations in a quantum circuit. Using Hadamard gates to introduce a superposition between helicity qubits, it enables simultaneous calculation of the + and − helicity states of each particle AND the s- and t-channel amplitudes for a 2→2 process

**Parton shower algorithm** calculates collinear emission for 2-step shower. While classical implementations must explicitly keep track of individual shower histories, our quantum algorithm constructs a wavefunction for the whole parton shower process with a superposition of all shower histories

First step towards a quantum computing algorithm to model the full collision event at LHC and demonstrate an excellent example of using quantum computers to model intrinsic quantum behaviour of the system
Future outlook

Slide credit: Steven Touzard’s talk given at CQT

- **Quantum Advantage**
- **Vision:** Solving real problems with speed-up; e.g. factorisation, chemistry, etc.
- **Today:** Noise Intermediate-Scale Quantum (NISQ) era
- **State of the art**

Preskill (2016)
Google Inc. (2019), Rigetti Computing (2018), etc
Quantum volume

Many factors contribute to the performance of the overall system
Future outlook

IBM Quantum Computing Roadmap

> 1000 qubits by 2023

Intermediate, near term goal: 1,121-qubit system by the end of 2023
Future outlook

Scaling IBM Quantum technology

<table>
<thead>
<tr>
<th>IBM Q System One (Released)</th>
<th>(In development)</th>
<th>Next family of IBM Quantum systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>2019 27 qubits <em>Falcon</em></td>
<td>2020 65 qubits <em>Hummingbird</em></td>
<td>2023 1,121 qubits <em>Condor</em></td>
</tr>
<tr>
<td>2021 127 qubits <em>Eagle</em></td>
<td>2022 433 qubits <em>Osprey</em></td>
<td>Path to 1 million qubits and beyond</td>
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<tr>
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<td></td>
<td>Large scale systems</td>
</tr>
</tbody>
</table>

Key advancement
- Optimized lattice
- Scalable readout
- Novel packaging and controls
- Miniaturization of components
- Integration
- Build new infrastructure, quantum error correction

Credit: StoryTK for IBM
Conclusions

• Quantum computing is an emergent and rapidly developing field with potential applications in variety of different areas

• Solutions to some of the most challenging problems in HEP may well be at the intersection of these two fields

• Current machines are excellent test beds for demonstrating proof-of-principle studies to make way for quantum revolution