



Quantum computing for simulating high energy collisions

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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



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Evolution of classical computer



Classical computers have come a long way since 1950s - size of machines (current size of transistor O(nm)) and complexity of computers

Quantum computing at a similar stage of development as classical computers in 1950s **Imperial College** ROYAL London SOCIETY 3

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

N qubits $\rightarrow 2^{N}$ dimensional Hilbert space

Power of quantum computing: this exponential increase in size of Hilbert space

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Quantum computing: Two classes/paradigms

Quantum Annealing

Quantum Gate Circuit



Find ground state of Hamiltonian through continuous-time adiabatic process

• Large number of 'noisy' qubits

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- Good for solving specific problems; for instance optimisation, machine learning.
- D-Wave specialises in quantum annealers



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

OUTPUT







Quantum gates: Hadamard

Hadamard gate

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- 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.

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

Circuit representation

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.

 $\text{CNOT}|00\rangle = |00\rangle,$ $\text{CNOT}|01\rangle = |01\rangle,$ $\text{CNOT}|10\rangle = |11\rangle,$ $\text{CNOT}|11\rangle = |10\rangle.$

Circuit representation



Γ1	0	0	0
0	1	0	0
0	0	0	1
0	0	1	0

Toffoli (CCNOT)

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- 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

$\mathrm{CCNOT} 000\rangle = 000\rangle,$	$\mathrm{CCNOT} 001\rangle = 001\rangle,$
$\mathrm{CCNOT} 100\rangle = 100\rangle,$	$\mathrm{CCNOT} 010\rangle = 010\rangle,$
$\operatorname{CCNOT} 110\rangle = 111\rangle,$	$CCNOT 111\rangle = 110\rangle.$

Circuit representation



Matrix representation

[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	0	1
0	0	0	0	0	0	1	0



Quantum supremacy?

Nature volume 574

- Google claimed quantum supremacy with 54qubit 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



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It's official: Google has achieved quantum supremacy () () () () () ()

PHYSICS 23 October 2019

By Daniel Cossins



Google's quantum computer is a record-breaker HANNAH BENET/Google



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Quantum computing in High Energy Physics





Track reconstruction at HL-LHC

- 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?









 b_{ij}

arXiv:1902.08324

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https://hep-qpr.lbl.gov

 $p_T \qquad p_T \quad 1$

0.1 rad

- 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 quaits))
- Use triplets (set of 3 hits); which triplets belong to the trajectory of a charged particle.

 T_i

 T_j

 (T_i, T_j) Minimise function O : equivalent to finding the ground -1-4state of the Hamiltonian ignored conflicts non-exhaustive *bij* = 0 $O(a, b, T) = \sum_{i=1}^{n} a_i T_i + \sum_i \sum_{j < i} b_{ij} T_i T_j$ $T_i,T_j\in\{0,1\}$ no shared hits ***** quadruplets a_i $b_{ij} = \mathbf{C} (> 0)$ weights, quality of individual encodes relationship between $b_{ij} = -S_{ij} (< 0)$ quality S triplets based on physics **T**triplets T_i properties b_{ij} T_i T_{i}

 $a_i = \alpha$

Minimising O = selecting the best triplets to form track candidates.

 $b_{ij} \qquad p_T \qquad \mu \qquad |$ $S(T_i, T_j) \qquad 12 \qquad 12$

Track reconstruction at HL-LHC

arXiv:1902.08324

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https://hep-qpr.lbl.gov

- 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



Higgs optimisation using D-Wave

- 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.



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 η^2

 ϕ^2



Higgs optimisation using D-Wave

Nature volume 550: 375–379(2017)

Map a signal vs background optimization problem to that of finding the ground state of a corresponding Ising spin model.





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

1098 active qubits



First application of D-Wave quantum annealing to a scenario in HEP



arXiv:2010.00046

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



Collision event at LHC



- Hard interaction + parton shower : can be described perturbatively + independent of non-perturbative processes.
- Most time consuming stages of event simulation THE ROYAL SOCIETY 18



Scattering amplitudes

- 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 N² 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





Equivalence between spinors and qubits

Helicity amplitude calculations based on manipulation of helicity spinors

Helicity spinors for massless states can be expressed as :

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

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

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

Equivalence between spinors and qubits

$$|p\rangle^{\dot{a}} = \sqrt{2E} \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} \qquad \longrightarrow \qquad |\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$

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

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A simple application of the helicity amplitude approach is the calculation of a $1 \rightarrow 2$ process



- 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 $10 \rightarrow 4$)

$$\mathcal{M}_{+} = -\sqrt{2} \frac{\langle p_{f}q \rangle [p_{\overline{f}}p]}{\langle qp \rangle}, \qquad \qquad \mathcal{M}_{-} = -\sqrt{2} \frac{\langle p_{f}p \rangle [p_{\overline{f}}q]}{[qp]}.$$

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 $1 \rightarrow 2$ helicity amplitude circuit

$$\mathcal{M}_{+} = -\sqrt{2} \frac{\langle p_{f}q \rangle [p_{\overline{f}}p]}{\langle qp \rangle}, \qquad \qquad \mathcal{M}_{-} = -\sqrt{2} \frac{\langle p_{f}p \rangle [p_{\overline{f}}q]}{[qp]}.$$



Figure 3: $gq\bar{q}$ vertex circuit. The amplitude for the process is calculated on the q_i qubits, which are controlled from the helicity register. The q_i qubits are then measured by the quantum computer.



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 $1 \rightarrow 2$ helicity amplitude circuit

$$\mathcal{M}_{+} = -\sqrt{2} \frac{\langle p_{f}q \rangle [p_{\overline{f}}p]}{\langle qp \rangle}, \qquad \qquad \mathcal{M}_{-} = -\sqrt{2} \frac{\langle p_{f}p \rangle [p_{\overline{f}}q]}{[qp]}.$$



Figure 3: $gq\bar{q}$ vertex circuit. The amplitude for the process is calculated on the q_i qubits, which are controlled from the helicity register. The q_i qubits are then measured by the quantum computer.

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 $1 \rightarrow 2$ helicity amplitude circuit

$$\mathcal{M}_{+} = -\sqrt{2} \frac{\langle p_{f}q \rangle [p_{\overline{f}}p]}{\langle qp \rangle}, \qquad \qquad \mathcal{M}_{-} = -\sqrt{2} \frac{\langle p_{f}p \rangle [p_{\overline{f}}q]}{[qp]}.$$



introduce a superposition between the helicity states $|+\rangle = |1\rangle$ and $|-\rangle = |0\rangle$

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 Hence, calculate the helicity of each particle involved simultaneously! ROYAL SOCIETY 26

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Run algorithm on:

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



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Run algorithm on:

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





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













$$\mathcal{M}_{t_{(++--)}} = 2\frac{\langle 34\rangle[21]}{\langle 13\rangle[31]}, \qquad -9 - \qquad \mathcal{M}_{t_{(+--+)}} = 2\frac{\langle 32\rangle[41]}{\langle 13\rangle[31]}.$$
$$\mathcal{M}_{s_{(+-+-)}} = 2\frac{\langle 24\rangle[31]}{\langle 12\rangle[21]}, \qquad \qquad \mathcal{M}_{s_{(+--+)}} = 2\frac{\langle 23\rangle[41]}{\langle 12\rangle[21]}$$





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!



- Proposed algorithm can be generalised to calculating helicity amplitudes for multi-particle final states.
- Using BCFW recursion formula, scattering amplitudes for massless partons can be reduced to combination of scalar products between helicity spinors

e.g. Parke-Taylor formula for $2 \rightarrow n$ gluon scattering process

$$\mathcal{A}_n[1^+\cdots i^-\cdots j^-\cdots n^+] = (-g_s)^{n-2} \frac{\langle ij \rangle^4}{\langle 12 \rangle \langle 23 \rangle \cdots \langle n1 \rangle}.$$

- The number of calculation qubits and helicity qubits needed in the algorithm both scale linearly with the number of final state particles.
- Each scalar product requires two spinor operations, the circuit depth scales linearly with number of scalar products.





Parton shower

- 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

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- 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: $p_i = zP$, $p_j = (1 z)P$
- Emission probabilities are calculated using collinear splitting functions, which at LO are given by:



Non-emission probability calculated using Sudakov factors

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

Probability of a splitting is given by,

$$\operatorname{Prob}_{k\to ij} = (1 - \Delta_k) \times P_{k\to ij}(z).$$

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Circuit for parton shower algorithm

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



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





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Results for parton shower algorithm





(b) Initial particle a quark.

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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





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 $2\rightarrow 2$ 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

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Future outlook

Slide credit: Steven Touzard's talk given at CQT







Performance of quantum computers



Future outlook



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

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Future outlook

Scaling IBM Quantum technology

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Credit: StoryTK for IBM



Conclusions

- Quantum computing 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



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