

A Quantum walk approach for simulating Parton showers

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Outline

- Brief intro to **Quantum Computing (QC)**
- intro to **Quantum Walk algorithms (QW)**
- **Parton shower** basics
- QW approach to parton showers
- Conclusions

Introduction to Quantum Computing

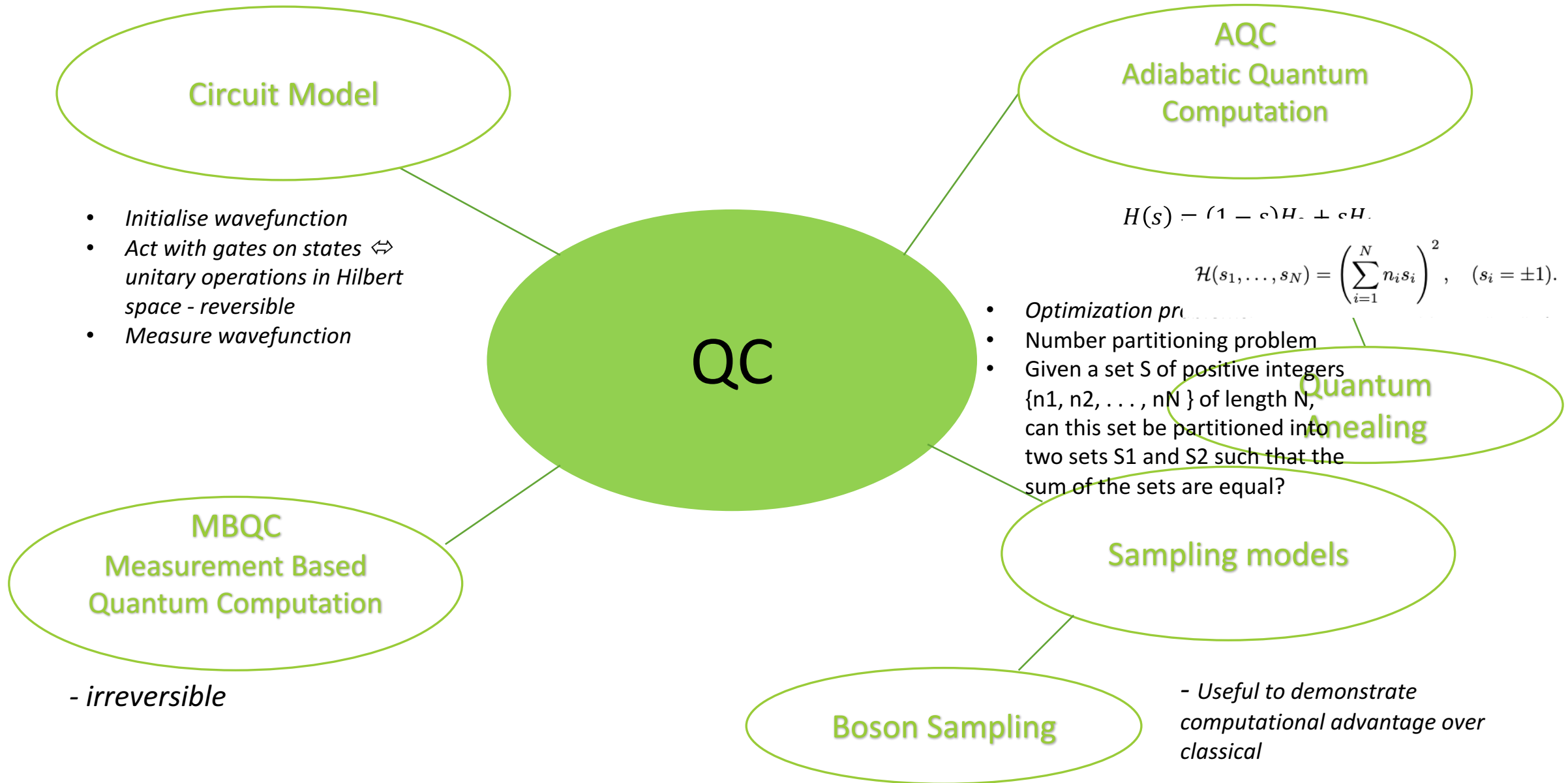
- **Bit :**

- Fundamental component of Classical Computation and Information
- Takes values 0 or 1

- **Qubit:**

- Two possible states $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow |\psi\rangle = \alpha|0\rangle + \beta|1\rangle$
- Specific parameterisation:
 - $|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)|1\rangle$

- *polarisations of photon, alignment of nuclear spin in magnetic field, two states of electron orbiting single atom*
- *N qubits – 2^N dim Hilbert space*



Quantum Gates

Single-qubit gates

NOT-gate (Pauli X gate)

$$\text{---} \boxed{X} \text{---} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Hadamard gate

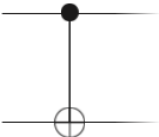
$$\text{---} \boxed{H} \text{---} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

S gate

$$\text{---} \boxed{S} \text{---} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

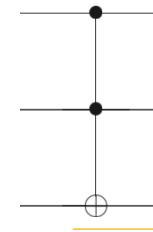
Multi-qubit gates

CNOT gate



$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

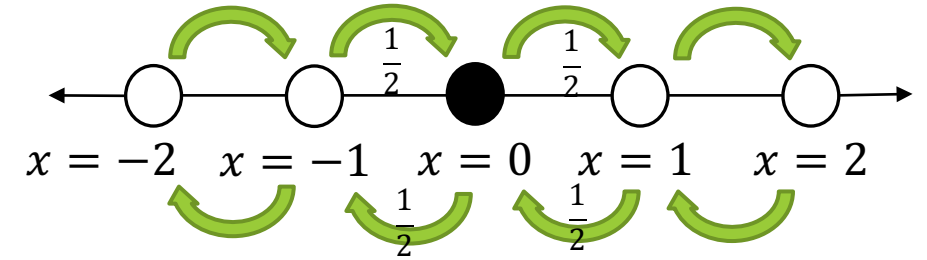
TOFFOLI gate



Can have universal sets e.g. {CNOT, H, T }

Solovay-Kitaev Th. Let G a finite subset of $SU(2)$ and $U \in SU(2)$. If the group generated by G is dense in $SU(2)$, then for any ε it is possible to approximate U to precision ε using $O(\log^4(1/\varepsilon))$ gates from G .
[Nielson Chuang.]

Intro to QW



Quantum walks (QW) are the quantum analog of the classical random walks

- using aspects of QM such as interference and superposition.

studied in two forms: Continuous-time (CT) QW and Discrete-Time (DT) QWs.

- various applications and studies e.g. in demonstrating exponential speedup over classical computation for a hitting time problem on a glued tree, quantum algorithms like the element distinctness problem, for like triangle finding etc. and also been employed to understand physical systems from phase transitions to modelling photosynthetic systems

[Chadrsekhar, Banerjee, Srikanth]

Continuous-time: directly encode the walk in the position Hilbert space, $\mathcal{H}_P$

Discrete-time: necessary to introduce additional coin Hilbert space to determine direction in which particle evolves in position space. Total Hilbert space given by: $\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_P$

CT QW

- Define CT classical random walk, quantize it introducing quantum amplitudes in place of classical probabilities
- Define CT classical random walk on position space spanned by vertex set V of graph G with edge set E , $G=(V,E)$
- Step of QW described by adjacency matrix, transform prob distribution over V

$$A_{j,k} = \begin{cases} 1 & (j,k) \in E, \\ 0 & (j,k) \notin E, \end{cases}$$

- For each pair (j,k) that belongs to
- Other important matrix is generator matrix

$$\mathbf{H}_{j,k} = \begin{cases} d_j \gamma & j = k \\ -\gamma & (j,k) \in E, \\ 0 & \text{otherwise} \end{cases}$$

- D_j = degree of vertex , γ is prob of transition between neighboring nodes per unit time
- Transition on graph G defined by solution to differential equation

$$\frac{d}{dt} p_j(t) = - \sum_{k \in V} \mathbf{H}_{j,k} p_k(t).$$

- where rate of change of probability of being at vertex j at time t , $p_j(t)$
- Solution:

$$p(t) = e^{-\mathbf{H}t} p(0).$$

[arXiv:1001.5326](https://arxiv.org/abs/1001.5326)

CT QW

- Replace probabilities by quantum amplitudes- $|j\rangle$ spans orthogonal position basis, introduce factor i

$$a_j(t) = \langle j|\psi(t)\rangle \text{ where } |j\rangle$$

$$i\frac{d}{dt}a_j(t) = \sum_{k \in V} \mathbf{H}_{j,k}a_k(t).$$

- CT QW $\Leftrightarrow$ Schrodinger eqn

$$i\frac{d}{dt}|\psi\rangle = \mathbf{H}|\psi\rangle.$$

- E.g. CT on line, basis states $|\psi_j\rangle$, where $j \in \mathbb{Z}$.

- Evolve system via $U(t) = \exp(-i\mathbf{H}t)$.

- Where Hamiltonian=generator matrix which evolves prob distribution given by

$$\mathbf{H}|\psi_j\rangle = -\gamma|\psi_{j-1}\rangle + 2\gamma|\psi_j\rangle - \gamma|\psi_{j+1}\rangle$$

DT QW (1D)

- Discrete time QW similar to the classical discrete random walk where the walk takes places on a position space with instruction from a coin operation
- Classical there is a coin flip, determines direction particles moves in, position shift moves the particle in corresponding direction
- Walk on line: 2 sided coin head and tails with equal prob determines movement to left or right
- In quantum case: coin flip replaced by quantum coin operation which creates a superposition of directions to which the particle evolves simultaneously

- Followed by unitary shift operation, repeated with large number of steps without intermediate measurements, retaining coherence of wavefunction
- Hilbert space give by
- Consider initial state defined by, particle at origin

$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p,$$

$$|\Psi_{in}\rangle = (\cos(\delta)|0\rangle + e^{i\eta} \sin(\delta)|1\rangle) \otimes |\psi_0\rangle,$$

-
- A general coin operation belongs U(2) defined by 4 parameters $B_{\zeta,\alpha,\beta,\gamma} = e^{i\zeta} e^{i\alpha\sigma_x} e^{i\beta\sigma_y} e^{i\gamma\sigma_z},$

- The shift operation is defined such that if the coin state is in $|0\rangle$ move right and if in $|1\rangle$ Move left i.e.

$$S = |0\rangle\langle 0| \otimes \sum_{j \in \mathbb{Z}} |\psi_{j-1}\rangle\langle \psi_j| + |1\rangle\langle 1| \otimes \sum_{j \in \mathbb{Z}} |\psi_{j+1}\rangle\langle \psi_j|.$$

- Entire operation given by

$$W_{\zeta,\alpha,\beta,\gamma} = S(B_{\zeta,\alpha,\beta,\gamma} \otimes \mathbb{1})$$

DT QW(1D)-dynamic structure

[arXiv:1003.4656](https://arxiv.org/abs/1003.4656)

Starting off with DT classical random walk

- For QW, information in coin state carried throughout making QW reversible. Lets see how this happens
- Describe wavefunction of state by 2-component vector of amplitudes being at position j at time t with left moving and right moving components $-p(j, t)$ $-p(j, t)$
- With symmetric structure, where $|\Psi(j, t)\rangle = \begin{pmatrix} \Psi_L(j, t) \\ \Psi_R(j, t) \end{pmatrix}$. article at position j and time t , prob at next time step given by equal measure from imm
- Consider a specific simple coin operation using $(0, \theta, -\frac{\pi}{2})$
- Subtracting $p(j, t)$ from both sides leads to difference equation corresponding to the Standard's classical diffusion eqn

$$B_{0, \theta, -\frac{\pi}{2}} = \begin{pmatrix} \cos(\theta) & -i \sin(\theta) \\ -i \sin(\theta) & \cos(\theta) \end{pmatrix}$$

- Write overall action of coin and conditional shift as

$$\begin{pmatrix} \Psi_L(j, t+1) \\ \Psi_R(j, t+1) \end{pmatrix} = \begin{pmatrix} \cos(\theta)a & -i \sin(\theta)a^\dagger \\ -i \sin(\theta)a^\dagger & \cos(\theta)a \end{pmatrix} \begin{pmatrix} \Psi_L(j, t) \\ \Psi_R(j, t) \end{pmatrix}, \quad (1)$$

- Where

$$\begin{aligned} a\Psi(j, t) &= \Psi(j+1, t), \\ a^\dagger\Psi(j, t) &= \Psi(j-1, t). \end{aligned}$$

A. Decoupled DT QW in Klein Gordon form

- Using (1) we can write out the individual LM and RM components at time t+1 as

$$\begin{aligned}\Psi_L(j, t+1) &= \cos(\theta)\Psi_L(j+1, t) - i\sin(\theta)\Psi_R(j-1, t), \\ \Psi_R(j, t+1) &= \cos(\theta)\Psi_R(j-1, t) - i\sin(\theta)\Psi_L(j+1, t).\end{aligned}$$

Can decouple Ψ_L and Ψ_R components to get

$$\begin{aligned}\Psi_R(j, t+1) + \Psi_R(j, t-1) &= \cos(\theta)[\Psi_R(j+1, t) + \Psi_R(j-1, t)], \\ \Psi_L(j, t+1) + \Psi_L(j, t-1) &= \cos(\theta)[\Psi_L(j+1, t) + \Psi_L(j-1, t)].\end{aligned}$$

- Using the definitions of the difference operator (*)
- If we subtract $2\Psi_R(j, t)$ from both sides of (1) we obtain a difference equation corresponding to the differential equation

$$\left[\cos(\theta) \frac{\partial^2}{\partial j^2} - \frac{\partial^2}{\partial t^2} \right] \Psi_R(j, t) = 2(1 - \cos(\theta))\Psi_R(j, t), \quad (2)$$

- Re-arranging this we see that this corresponds to the Klein-Gordon equation
- Where

So that each component of the DT QW has the relativistic character of a free spin-0 particle

$$\begin{aligned}c &\equiv \sqrt{\cos(\theta)}, \\ \mu = \frac{mc}{\hbar} &\equiv \sqrt{2[\sec(\theta) - 1]}.\end{aligned}$$

$$m \equiv \sqrt{\frac{2[\sec(\theta) - 1]}{\cos(\theta)}}.$$

$$\begin{aligned} (*) \quad \nabla_t &= \frac{\Psi(j, t + \frac{h}{2}) - \Psi(j, t - \frac{h}{2})}{h}. \\ \nabla_t^2 &= \frac{1}{h} \times \frac{[\Psi(j, t+1) - \Psi(j, t)] - [\Psi(j, t) - \Psi(j, t-1)]}{h} \\ &= \frac{(\Psi(j, t+1) - 2\Psi(j, t) + \Psi(j, t-1))}{h^2}, \\ h=1, \rightarrow \partial_t^2\end{aligned}$$

B. Decoupled DT QW in Schrodinger form

- KG eqn's can then be transformed into the Schrodinger equation
- Transform (2)-second order in time-into system of 2 coupled differential equations first order in time using ansatz

$$\Psi_R = \varphi_R + \chi_R, \quad i\hbar \frac{\partial \Psi_R}{\partial t} = \sqrt{2[1 - \cos(\theta)]} (\varphi_R - \chi_R), \quad (3)$$

- Can show that the following coupled eqns are equivalent to (2)

$$i\hbar \frac{\partial \varphi_R}{\partial t} = -\frac{\hbar^2}{2\sqrt{\frac{2[\sec(\theta)-1]}{\cos(\theta)}}} \Delta(\varphi_R + \chi_R) + \sqrt{2[1 - \cos(\theta)]} \varphi_R, \quad (4)$$

$$i\hbar \frac{\partial \chi_R}{\partial t} = \frac{\hbar^2}{2\sqrt{\frac{2[\sec(\theta)-1]}{\cos(\theta)}}} \Delta(\varphi_R + \chi_R) - \sqrt{2[1 - \cos(\theta)]} \chi_R, \quad (5)$$

- Subtracting (5) from (4), and re-arranging (3)

$$i\hbar \frac{\partial}{\partial t} (\varphi_R - \chi_R) = -\frac{\hbar^2}{\sqrt{\frac{2[\sec(\theta)-1]}{\cos(\theta)}}} \Delta(\varphi_R + \chi_R) + \sqrt{2[1 - \cos(\theta)]} (\varphi_R + \chi_R),$$

$$i\hbar \frac{\partial}{\partial t} \left(\frac{i\hbar}{\sqrt{2[1 - \cos(\theta)]}} \frac{\partial \Psi_R}{\partial t} \right) = -\frac{\hbar^2}{\sqrt{\frac{2[\sec(\theta)-1]}{\cos(\theta)}}} \Delta \Psi_R + \sqrt{2[1 - \cos(\theta)]} \Psi_R,$$

$$\frac{1}{\sqrt{2[1 - \cos(\theta)]}} \frac{\partial^2 \Psi_R}{\partial t^2} = \frac{1}{\sqrt{\frac{2[\sec(\theta)-1]}{\cos(\theta)}}} \Delta \Psi_R - \sqrt{2[1 - \cos(\theta)]} \Psi_R,$$

$$\frac{1}{\sqrt{2[\sec(\theta) - 1] \cos(\theta)}} \frac{\partial^2 \Psi_R}{\partial t^2} = \frac{\sqrt{\cos(\theta)}}{\sqrt{2[\sec(\theta) - 1]}} \Delta \Psi_R - \sqrt{2[\sec(\theta) - 1] \cos(\theta)} \Psi_R.$$

Thus we get:

$$\left(\frac{1}{\cos(\theta)} \frac{\partial^2}{\partial t^2} - \Delta \right) \Psi_R = -2[\sec(\theta) - 1] \Psi_R.$$

B. Decoupled DT QW in Schrodinger form

- So looking at (4) and (5) they can be combined by introducing the column vector

$$\Psi_R = \begin{pmatrix} \varphi_R \\ \chi_R \end{pmatrix}$$

- And using the 4 2x2 matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

- with algebraic relations $\sigma_k^2 = \mathbb{1}$, $\sigma_k \sigma_l = \sigma_l \sigma_k = i \sigma_m$, $k, l, m = 1, 2, 3$ – in a cycle.

- We can form the schrodinger-type equation

$$\left(i\hbar \frac{\partial}{\partial t} - \hat{\mathbf{H}}_R \right) \Psi_R = 0,$$

- Where

$$\hat{\mathbf{H}}_R = (\sigma_3 + i\sigma_2) \frac{\hat{P}^2 \sqrt{\cos(\theta)}}{2\sqrt{2[\sec(\theta) - 1]}} + \sigma_3 \sqrt{2[1 - \cos(\theta)]}.$$

- And $\hat{P} = i\hbar \nabla$

- And we can obtain a similar eqn for Ψ_L

- We have found that each component of DT QW has a structure similar to KG eqn which can also be written as coupled schrodinger eqn
- So a DT QW can be described as a coupled form of the CT QW driven by 2 Hamiltonians $\hat{\mathbf{H}}_L$ and $\hat{\mathbf{H}}_R$

So what + how?

[arXiv:quant-ph/0303081](https://arxiv.org/abs/quant-ph/0303081)

- Both discrete and continuous QWs have natural implementations within quantum computers
- A very well studied type of DT QW implemented on a quantum computer is the Hadamard walk coin operation is given by the hadamard gate

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

- Again the coin space is defined in this 1D walk by the computational basis of a qubit i.e. $|0\rangle$ and $|1\rangle$
- Whilst position states defined by integers
- If we start with initial state $|\uparrow\rangle \otimes |0\rangle$

- a single step first applies the coin operator and then applies a shift

$$\begin{aligned} |\uparrow\rangle \otimes |0\rangle &\xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle \\ &\xrightarrow{S} \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle + |\downarrow\rangle \otimes |-1\rangle). \end{aligned}$$

- Measuring in the standard coin basis gives with probability $\frac{1}{2}$

$$\{|\uparrow\rangle \otimes |1\rangle, |\downarrow\rangle \otimes |-1\rangle\}$$

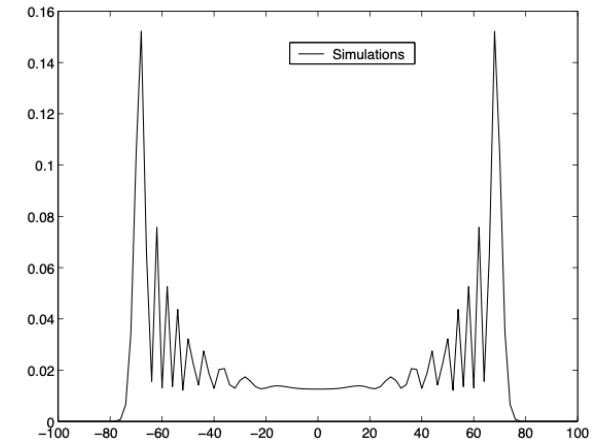
- If we continued by measuring after each iteration we would get the classical random walk on the line where the limiting distribution approaches a gaussian distribution with mean zero and variance

$T \backslash i$	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{3}{8}$		$\frac{3}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{1}{4}$		$\frac{3}{8}$		$\frac{1}{4}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{5}{32}$		$\frac{5}{16}$		$\frac{5}{16}$		$\frac{5}{32}$		$\frac{1}{32}$

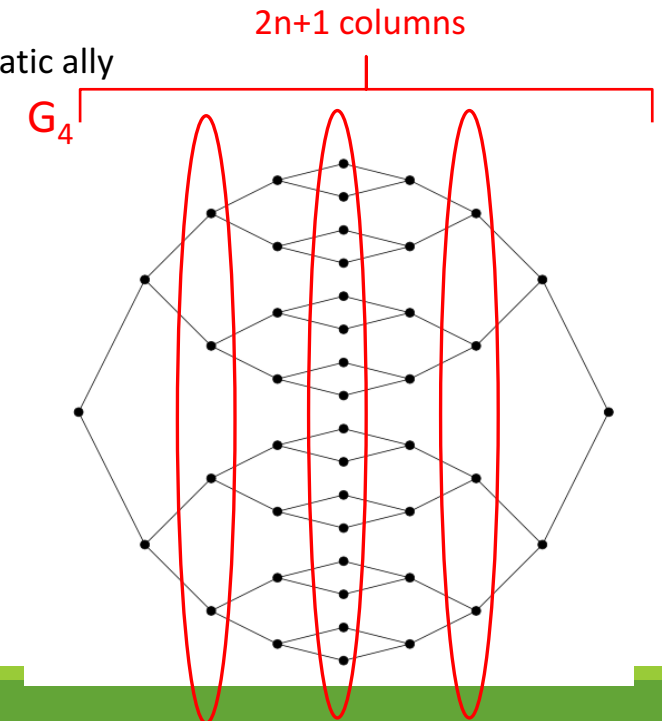
$T \backslash i$	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$	0	$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{17}{32}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{5}{32}$		$\frac{1}{32}$

- In the QW i.e. without measurement the interference will cause a radically different behavior of the QW
- Just by considering the initial state after 3 steps we get, asymmetry with respect to different positions

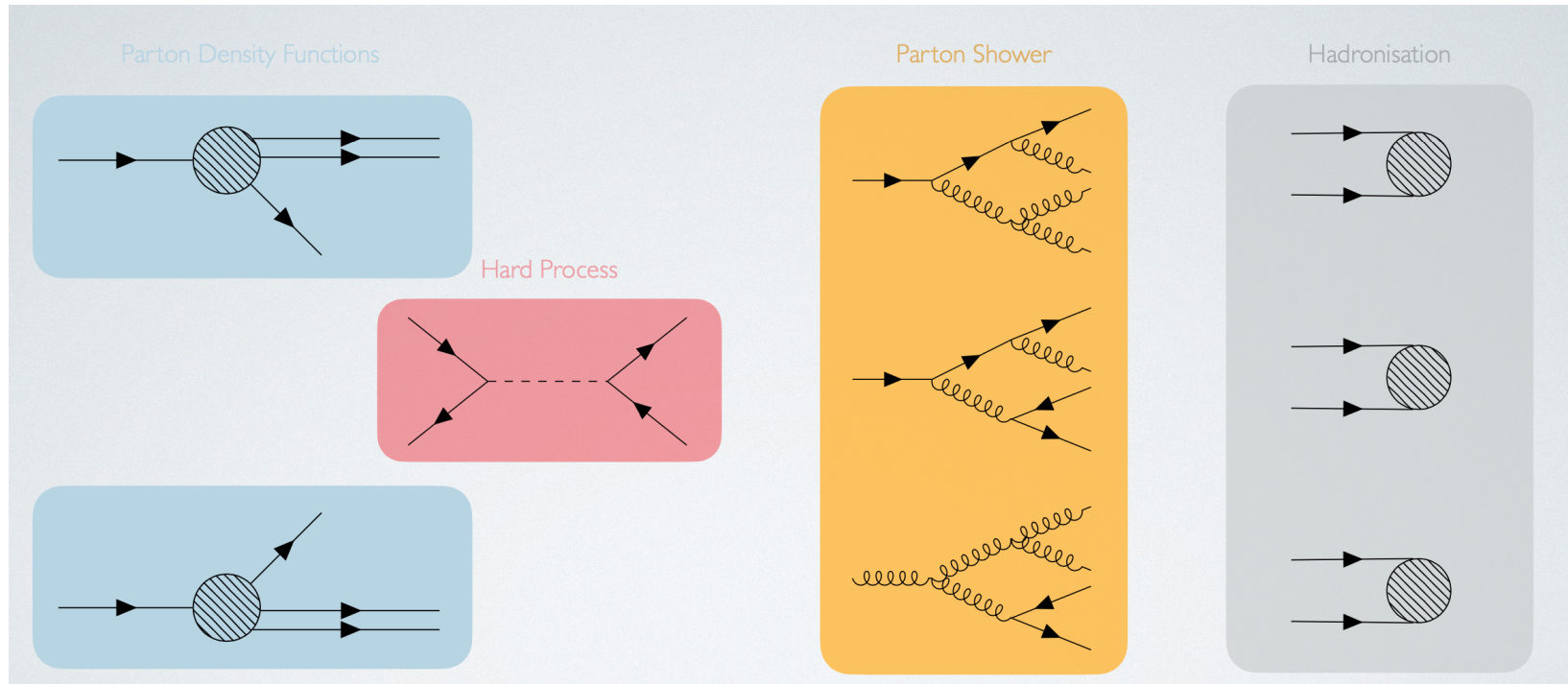
$$\begin{aligned}
 |\Phi_{in}\rangle &\xrightarrow{U} \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle - |\downarrow\rangle \otimes |-1\rangle) \\
 &\xrightarrow{U} \frac{1}{2}(|\uparrow\rangle \otimes |2\rangle - (|\uparrow\rangle - |\downarrow\rangle) \otimes |0\rangle + |\downarrow\rangle \otimes |-2\rangle) \\
 &\xrightarrow{U} \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |3\rangle + |\downarrow\rangle \otimes |1\rangle + |\uparrow\rangle \otimes |-1\rangle \\
 &\quad - 2|\downarrow\rangle \otimes |-1\rangle - |\downarrow\rangle \otimes |-3\rangle). \quad (16)
 \end{aligned}$$



- Starting with a symmetric initial state i.e. superposition of coin states, the hadamard walk after 100 steps results in the following distribution
- This has a variance of which gives an expected distance from the original of $\sim$ the QW propagates quadratic ally faster
- Another example where there is speed up in QWs is in **expected hitting time** in graphs, i.e. the time it takes for a random walk to reach a point T on a graph from point S.
- a graph G_n of n -level binary trees glued together at their leaves for example G_4
- For classical case it was found that the prob of reaching column $2n$ in polynomial time in n was exponentially small in n
- Whilst implementing the walk as CT QW with $2n+1$ vertices it was found that speed of propagation on infinite line was linear in time T



Parton Shower Quantum Algorithm?



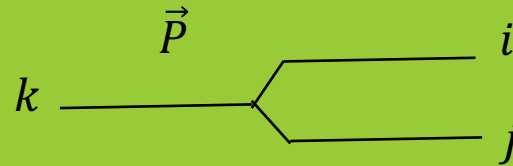
- Markov chain algorithm $\rightarrow$ Random walk?
- Previous Quantum algorithms for parton showers: arXiv:1904.03196v2

- Monte Carlo event generators are used to simulate high energy collisions at the LHC
- simulation is split into several stages.
 - hard-scattering of incoming partons stemming from colliding protons
 - Producing highly energetic states which then decay.
- Going to lower energetic scales, the incoming hadrons as well as the outgoing particles radiate lighter particles, like gluons and photons
- they are able to radiate further, producing a cascade of particles which realised through the parton shower algorithm
- Evolve down energy scales leading to hadronization

Parton Shower-Outline

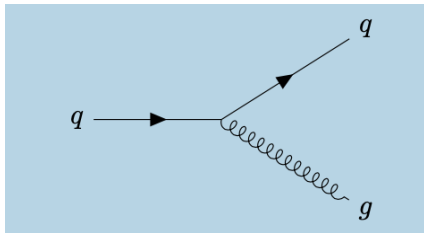
- We consider a discrete, collinear toy QCD model comprising one gluon and one quark flavour
- Only consider collinear splittings, not keeping track of kinematics which means can also be encoded in available qubit-restricted quantum computers

Collinear condition:

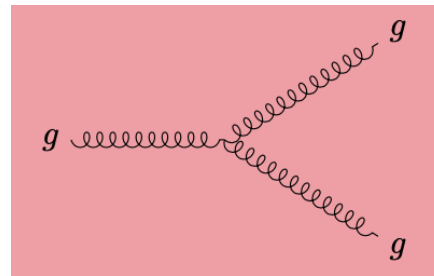


$$p_i = zP,$$

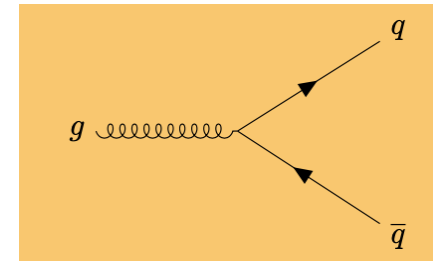
$$p_j = (1 - z)P$$



$$P_{q \rightarrow qg}(z) = C_F \frac{1 + (1 - z)^2}{z},$$



$$P_{g \rightarrow gg}(z) = C_A \left[2 \frac{1 - z}{z} + z(1 - z) \right],$$



$$P_{g \rightarrow q\bar{q}}(z) = n_f T_R (z^2 + (1 - z)^2),$$

Parton Shower - outline

- Sudakov factors are used to determine whether an emission occurs

$$\Delta_{i,k}(z_i, z_k) = \exp \left[-\alpha_s^2 \int_{z_1}^{z_2} P_{k'}(z') dz' \right], \quad \Delta_{tot}(z_1, z_2) = \Delta_g^{n_g}(z_1, z_2) \Delta_q^{n_q}(z_1, z_2) \Delta_{\bar{q}}^{n_{\bar{q}}}(z_1, z_2),$$

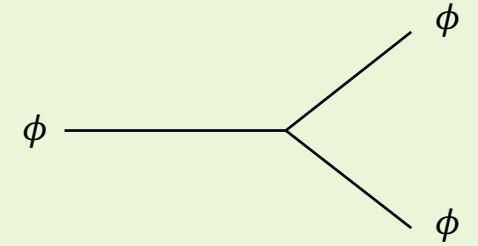
- The overall splitting probability is given by the Sudakovs, and the splitting functions such that

$$Prob_{k \rightarrow ij} = (1 - \Delta_k) \times P_{k \rightarrow ij}(z)$$

- Shower evolution is determined by exponentially decreasing the evolution variable z with number of steps

QW approach to PS

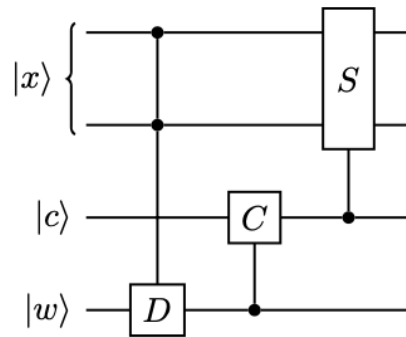
$$\phi \rightarrow \phi\phi: P_{\phi \rightarrow \phi\phi}$$



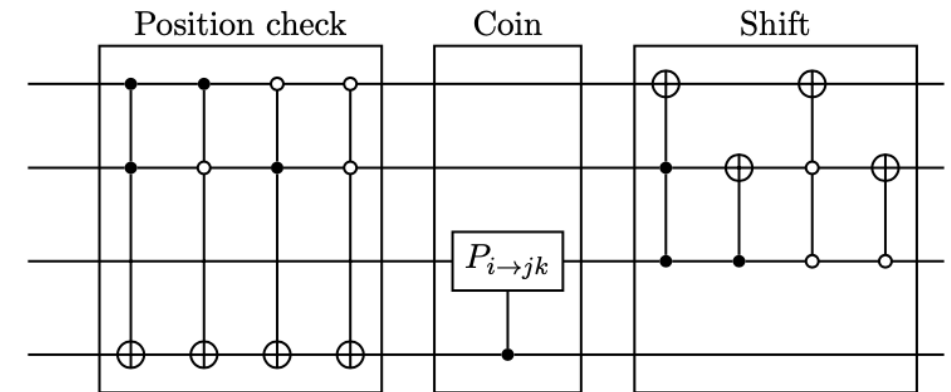
- consider an initial simple model with a single particle type, ϕ
- probability of emission in the QW formalism is encoded within the coin operation given by

$$C = \begin{pmatrix} \sqrt{1 - P_{jk}} & -\sqrt{P_{jk}} \\ \sqrt{P_{jk}} & \sqrt{1 - P_{jk}} \end{pmatrix}$$

- define the position Hilbert space where basis states given by number of phi particle, $|n_\phi\rangle$
- Where $n_\phi \in \mathbb{Z}^*$



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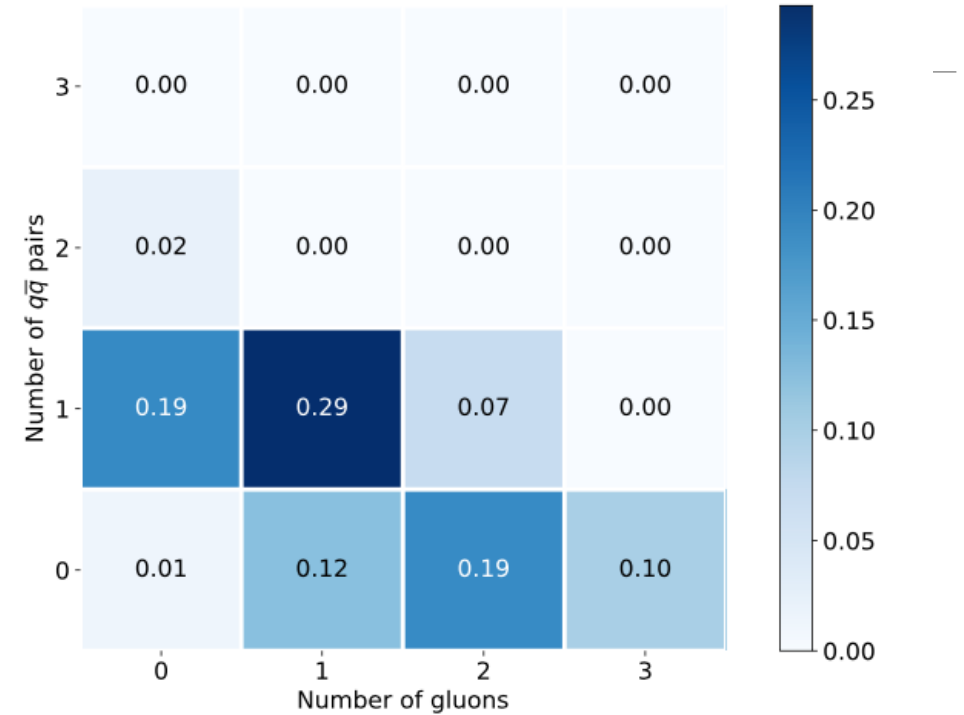


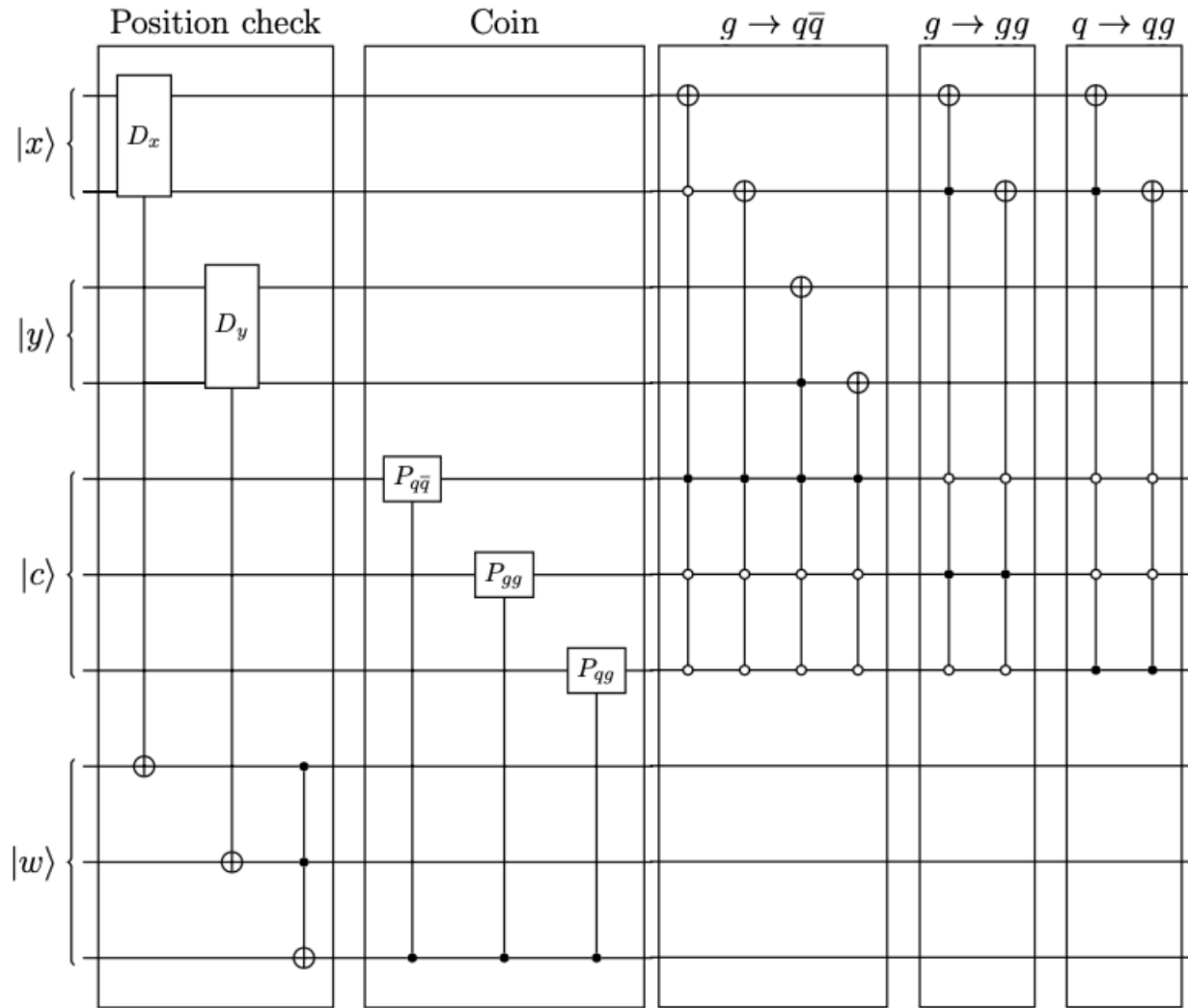
QW approach to PS

- Now we consider a 2 dimensional model considering simulation of both quarks and gluons
- enlarge the coin Hilbert space to encode 3 types of splitting probabilities given by

$$P_{ij} = (1 - \Delta_k) \times P_{k \rightarrow ij}(z)$$

- S operator now updates either the gluon number or quark number on each respective axis conditioned on the states of the coin space

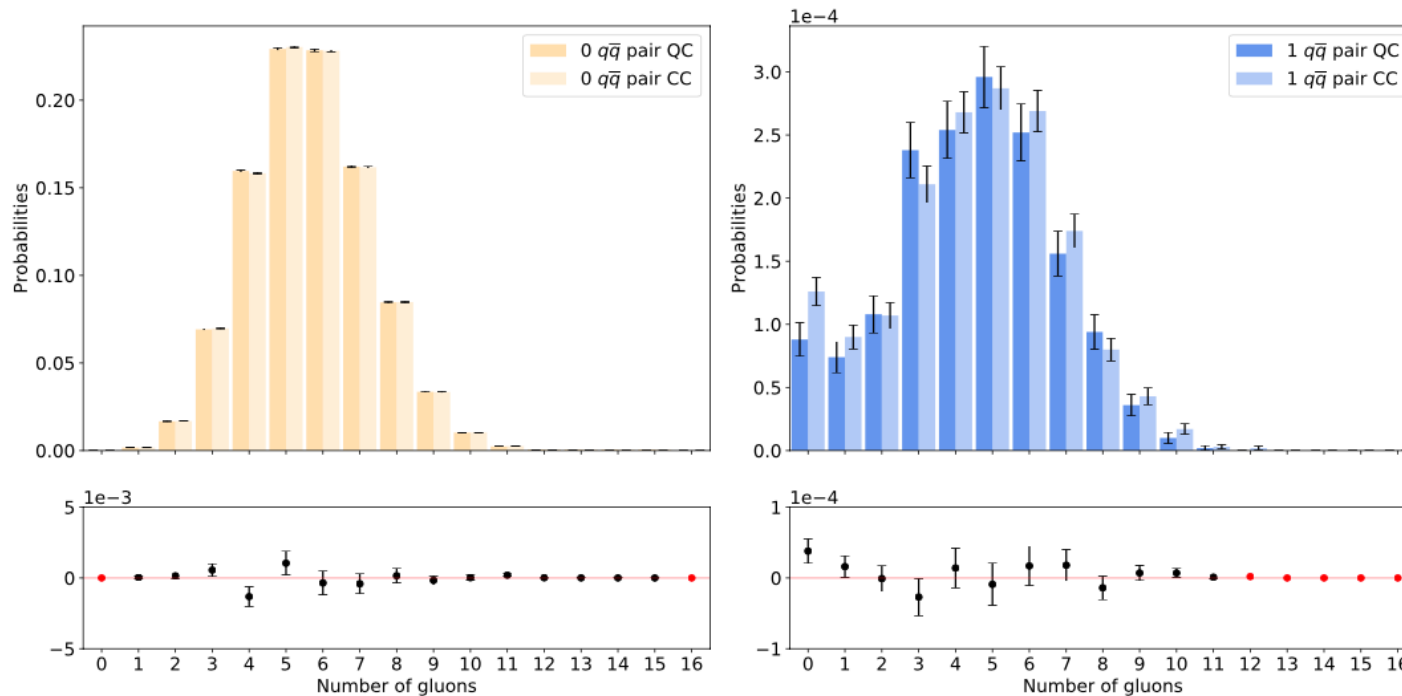




QW approach to PS

- algorithm was implemented on IBM Q Quantum Simulator, using 16 qubits simulating 31 shower steps
- The algorithm scales as $2\log_2(N + 1) + 4$
- By reframing the parton shower in the quantum walk framework greatly increases number of shower steps possible to simulate in comparison to previous quantum algorithms, whilst also using less volume

QW approach to PS



- Probability distribution of the number of gluons measured at the end of the 31-step parton shower for the classical and quantum algorithms
- zero quark anti-quark pairs (left) and exactly one quark anti-quark pair (right)
- run on the IBMQ 32-qubit quantum simulator for 500,000 shots, and the classical algorithm has been run for 10^6 shots.

Summary

Presented a dedicated quantum algorithm for the simulation of parton shower in high energy collisions

- Demonstrated the ability to calculate shower histories of parton shower in full superposition
- Found that reframing parton shower in as a quantum walk algorithm provides a more natural and efficient approach to simulating parton showers

In the future:

- Would like to introduce kinematics which will vastly increase realism of the quantum algorithm. Algorithm presented here can be seen as a first step towards a full and realistic quantum simulation of a high energy collision process.