Quantum Walk on FRET Networks

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Abstract In this section, we introduce the basics of quantum walk algorithm and its applications. Quantum walk is a natural extension of the concept of random walk in quantum way; therefore, the results obtained from the discussion are considered as the results by Quantum Computation. In principle, we can expect a certain type of the computation would be boosted. There are a variety of phenomena in Quantum walks, and much broader outcomes are often obtained than those from classical random walk. Such famous examples include quantum search algorithms and quantum simulations. In this article, we introduce a quantum simulation of QCD parton shower algorithm appearing in particle physics.

1 Introduction of Quantum Walk

In this section, we introduce the Quantum Walk algorithm as an extended version of Classical Random Walk.

1.1 Classical Random Walk

Let us begin with a traditional classical random walk on the integer points of a 1-dimensional line. We call the object which will move around on the line as "walker" and the movement of the "walker" is determined step-by-step randomly according to the given probability p. At each step, the "walker" can move to the left or the right integer points next to the current point with the probability of p and $1 - p$, respectively. We consider the same procedure t times repeated, then although we cannot predict the location of the "walker" n at the time t we can compute the probability of it.

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H. Suzuki et al. (eds.), *Photonic Neural Networks with Spatiotemporal Dynamics*,
https://doi.org/10.1007/978-981-99-5072-0_7

Suppose at $t = 0$ the "walker" starts at $n = 0$, then the probability that he is at n at the time t is given by

$$P(t, n) = {}_tC_{\frac{t+n}{2}} 2^{-t}, \tag{1}$$

where ${}_tC_n = t!/(t-n)!n!$.

An important consideration here is that we can consider the "path", in other words, "history", the set of the positions of the "walker" at all the time steps before the ending time t, $\{n_{t'} | 0 \leq t' \leq t\}$, and that we can compute the probability of the appearance of a certain "path". For this example, each "path" appears at the probability of 2^{-t}. The above probability is given by counting the number of possible "paths" ending at position n. For the generic p, the appearance probability of each "path" becomes $p^{n_+}(1-p)^{n_-}$, where $n = n_+ - n_-$ and $t = n_+ + n_-$.

For the random walk, we can compute the average $\mu = \langle n \rangle$ and the variance $\sigma^2 = \langle n^2 \rangle - \mu^2$ as $\mu = (2p-1)t$ and $\sigma^2 = p(1-p)t$. Especially, the standard deviation σ scales as $O(\sqrt{t})$. The asymptotic probability distribution becomes

$$\lim_{t\to\infty} P(X_t/\sqrt{t} \leq x) = \int_{-\infty}^{x} f(y)\mathrm{d}y, \quad \text{where,} \quad f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2} \right].$$

1.2 Quantum Walk

In classical random walk, we can predict the probability of the position of the walker at time t by considering all the possible "paths" of the walker and computing the probability of the "path". We want to consider the quantum version of the corresponding system. The most important property of the quantum system is that we can consider the superposition of the states. Thus, we in the end want to consider the superposition of the "paths".

The dynamics of a quantum walk can be described using a quantum mechanical formalism [1, 2]. The state of the particle on several nodes can be represented by a quantum state vector, which evolves according to a unitary operator. One can imagine that each node is lined on a 1-dimensional line, labeled with an integer n. Note that the following discussion is not restricted to the nodes lined in a line, but are valid as long as we can label the node with n, for example, in the case that the nodes are vertices on a graph. The position of the "walker" is described by the quantum state $|n\rangle$, which spans the position Hilbert space $\mathcal{H}_P = \{|n\rangle | n \in \mathbb{Z}\}$. Furthermore, for each node, we assume there are two discrete states, like spin up and down. This Hilbert space is denoted as $\mathcal{H}_C$, and we can label the two states with $\{|\uparrow\rangle, |\downarrow\rangle\}$, $\{|0\rangle, |1\rangle\}$, $\{|L\rangle, |R\rangle\}$, $\{|+\rangle, |-\rangle\}$, or often $\{|H\rangle, |T\rangle\}$, which means "head" and "tail". The coined operator is acting on this Hilbert space. The whole Hilbert space considered is the product of the two Hilbert spaces $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C$, where the dimension of the Hilbert space is

the product of the dimensions of $\mathcal{H}_P$ and $\mathcal{H}_C$. The quantum state $|\psi(t)\rangle$ at each time step t is given by

$$|\psi(t)\rangle = \sum_n \left[\psi_{n,+}(t)|n,+\rangle + \psi_{n,-}(t)|n,-\rangle\right],$$

where

$$\sum_n \left[|\psi_{n,+}(t)|^2 + |\psi_{n,-}(t)|^2\right] = 1.$$

The evolution of the quantum state $|\psi(t)\rangle$ is described by the following algorithms:

1. Initial state: The particle is initialized at some node on the graph with a specific quantum state $|\psi(0)\rangle$:

$$|\psi(0)\rangle = \sum_{n,s_n=\pm} \psi_{n,s_n}(0)|n,s_n\rangle.$$

   For example, $\psi_{0,0}(0) = 1$, otherwise 0.

2. Quantum coin operation: The particle's state is modified by a quantum coin operator $C \in U(2)$, which is a 2-dimensional unitary operator that acts on a coin state $|c\rangle = \alpha_+|+\rangle + \alpha_-|-\rangle \in \mathcal{H}_C$. Explicitly, $|c'\rangle = C|c\rangle$ can be described by

$$C = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, |c'\rangle = \begin{pmatrix} \alpha'_- \\ \alpha'_+ \end{pmatrix}, |c\rangle = \begin{pmatrix} \alpha_- \\ \alpha_+ \end{pmatrix}.$$

3. Conditional shift: The particle's position is then shifted according to the coin operation. For each node, there is a corresponding shift operator that acts on the state of the particle. The shift operator is often defined as

$$S = \sum_j |j\rangle\langle j-1| \otimes |+\rangle\langle +| + |j\rangle\langle j+1| \otimes |-\rangle\langle -| = S_+ \otimes P_+ + S_- \otimes P_-,$$

   where $|j\rangle$ represents the state of the particle at node j, and $\otimes$ denotes the tensor product.
4. Total evolution: The total evolution of the quantum walk for each time step is given by the operator:

$$U = S(I \otimes C),$$

   where C is the coin operator in $\mathcal{H}_C$, and I is the identity operator in $\mathcal{H}_P$. The total evolution of the quantum walk over t time steps is given by the product of U taken over t steps, U^t. The final form of the quantum state $|\psi(t)\rangle$ is obtained

as follows:

$$|\psi(t)\rangle = U^t|\psi(0)\rangle.$$

These equations describe the basic dynamics of a quantum walk on a line. By choosing appropriate initial states, coin operators, and graph structures, quantum walks can be used to solve various problems in quantum computing, such as search and sampling.

Explicit form of the U operator is given by

$$U = S(I \otimes C) = \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & 0 & P_- & 0 & \cdots \\ \cdots & P_+ & 0 & P_- & \cdots \\ \cdots & 0 & P_+ & 0 & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & C & 0 & 0 & \cdots \\ \cdots & 0 & C & 0 & \cdots \\ \cdots & 0 & 0 & C & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & 0 & P & 0 & \cdots \\ \cdots & Q & 0 & P & \cdots \\ \cdots & 0 & Q & 0 & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix},$$

where

$$P = P_-C = \begin{pmatrix} a & b \\ 0 & 0 \end{pmatrix}, Q = P_+C = \begin{pmatrix} 0 & 0 \\ c & d \end{pmatrix}, C = P + Q.$$

Acting U once provides the probability of finding the walker at $(1, \pm 1)$ as $|P\psi_0|^2$ and $|Q\psi_0|^2$, respectively, so $|a|^2 + |c|^2 = 1$ gives the similar relation of the classical random walk system. However, if we consider more than two steps, U^t essentially provide $\psi_n(t)$ as a coherent sum of the amplitudes corresponding to the possible paths to reach the point (t, n) from $(0, 0)$ as in Fig. 1. It is conceptually happening for the quantum system when we don't observe the intermediate states and only observe the final wave function at time t.

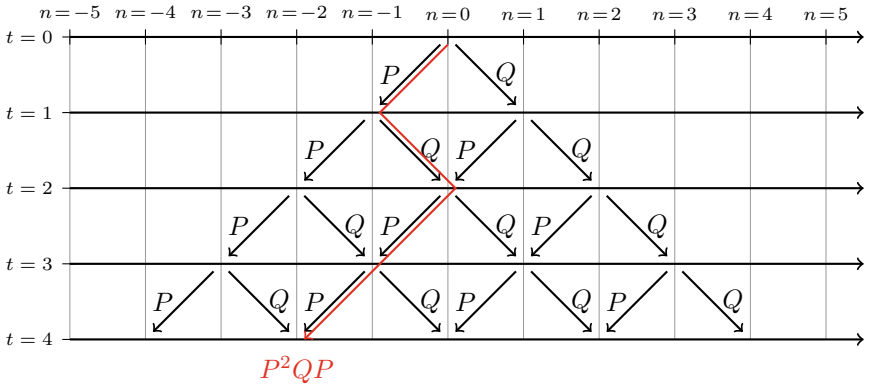

Fig. 1 Quantum walk paths. An example path is denoted in red line and the corresponding amplitude is obtained by the products of P and Q acting on the initial state $\psi_0(0)$

For an example discussion, the coin operator is often chosen to be a Hadamard coin operator H,

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

which puts the coin into an equal superposition of $|+\rangle$ and $|-\rangle$ states. For example, the coin state obtained by H acting on $|+\rangle$ is given by $H|+\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$.

Here, in this setup, for the coin operator in general we can consider only the element of $SU(2)$, since the overall phase is not relevant in quantum computation. Thus, the variety of coin operator is parameterized with 3-dimensional real parameters, $a, b \in \mathbb{C}$ satisfying $|a|^2 + |b|^2 = 1$, and

$$C = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} \sqrt{1-|b|^2} & b \\ -b & \sqrt{1-|b|^2} \end{pmatrix}.$$

The last line can be obtained when a and b are restricted being real.

With this parameterization, it is known that the asymptotic probability distribution of X_t (the position of the walker at time t) in the Quantum Walk with the initial state $\psi_0(0) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$, and $\psi_n(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ $(n \neq 0)$ is given by the following [1, 2]:

$$\lim_{t\to\infty} P(X_t/t \leq x) = \int_{\infty}^{x} f(y) I_{(-|a|,|a|)}(y) \mathrm{d}y,$$

$$f(x) = \frac{\sqrt{1-|a|^2}}{\pi(1-x^2)\sqrt{|a|^2-x^2}} \left[1 - (|\alpha|^2 - |\beta|^2 + \frac{2Re[a\alpha b^* \beta^*]}{|a|^2})x \right],$$

where $I_A(y)$ is the compact support function giving $I_A(y) = 1$ for $y \in A$, and otherwise 0. Especially, most of the distributions accumulate around $x \sim \pm|a|$. The important fact for the Quantum Walk is that the standard deviation σ scales as $O(t)$ not $O(\sqrt{t})$, which would be advantageous for faster search algorithm and for generating samples far from initial states (Fig. 2).

1.3 Quantum Walk on FRET Networks

In the previous chapter, a mathematical model of the FRET network is introduced, where the reactions among the excited states and the ground states in an array of Quantum Dots (QDs) are considered. As a physical system, it should be more appropriate to treat it as a quantum system as a whole. We here introduce a way to include parts of the quantum effects, the interference effects, to the mathematical model of the FRET network.

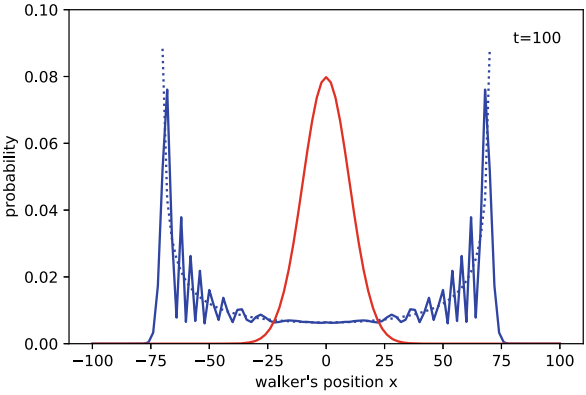

Fig. 2 An example probability distribution of the walker at time $t = 100$ in Quantum Walk (blue). The corresponding asymptotic probability of the Quantum Walk (blue-dashed) and the Classical Random Walk (red) are also shown for comparison

For simplicity, we consider the case where the interactions occur only between the QDs which are next to each other in the 1-dimensional array of QDs. That means, we consider the case $k_{nm} \neq 0$ only when $m = n + 1$, and otherwise $k_{nm} = 0$. We also assume the spontaneous decay process is negligible, i.e. $k_n = 0$. The resulting master formula is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} P_n(t) = -k_{n,n+1} P_n(t) + k_{n-1,n} P_{n-1}(t).$$

Changing the continuous time to discrete time Δt,

$$P_n(t + \Delta t) = \left(1 - k^{\mathrm{FRET}}_{n,n+1} \Delta t\right) P_n(t) + k^{\mathrm{FRET}}_{n-1,n} \Delta t \, P_{n-1}(t). \tag{2}$$

Since the sum of the probability of all the possible configurations is conserved, we can describe this system as a unitary transformation acting on the vector in the Hilbert space that consists of the direct product of the Hilbert space representing n QDs $\{|n\rangle\}$ and that representing excited/non-excited states $\{|+\rangle, |-\rangle\}$ for each QD, which is originally in 2^N dimensions but restricted to the $2N$ dimensions since the number of excited states is restricted to one or zero. Thus, hot vector representation can be represented as $\psi_{0_1,\ldots,0_{n-1},1_n,0_{n+1},\ldots,0_N} |0_1, \ldots, 0_{n-1}, 1_n, 0_{n+1}, \ldots, 0_N\rangle = \psi_{n,+}(|n\rangle \otimes |+\rangle)$. For each step, the FRET interaction is acting as the transition from $|n\rangle \otimes |+\rangle \to |n + 1\rangle \otimes |+\rangle$. Thus, to reproduce the correct transition probability using the coin operator in the QW algorithm, we can take $b = \sqrt{k^{\mathrm{FRET}} \Delta t}$. The explicit form of C is given as

$$C = \begin{pmatrix} \sqrt{1 - k^{\mathrm{FRET}} \Delta t} & \sqrt{k^{\mathrm{FRET}} \Delta t} \\ -\sqrt{k^{\mathrm{FRET}} \Delta t} & \sqrt{1 - k^{\mathrm{FRET}} \Delta t} \end{pmatrix},$$

and for this case we can take the shift operator $S' = S_+ \otimes |+\rangle\langle+| + S_0 \otimes |-\rangle\langle-|$. The corresponding U operator is given by

$$U' = S'(I \otimes C) = \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & P_- & 0 & 0 & \cdots \\ \cdots & P_+ & P_- & 0 & \cdots \\ \cdots & 0 & P_+ & P_- & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & C & 0 & 0 & \cdots \\ \cdots & 0 & C & 0 & \cdots \\ \cdots & 0 & 0 & C & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} = \begin{pmatrix} \vdots & \vdots & \vdots & \\ \cdots & P & 0 & 0 & \cdots \\ \cdots & Q & P & 0 & \cdots \\ \cdots & 0 & Q & P & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix}.$$

With this unitary operator, we can reproduce the relationship among the amplitude and the probability for one time step, which we assume to be the case when at each step we observe the configuration. For more time steps, we should get

$$\psi(t) = (U')^t \psi(0) = \begin{pmatrix} & \vdots & \vdots & \vdots & \\ \cdots & P^t & 0 & 0 & \cdots \\ \cdots & \sum_{i=0}^{t-1} P^i Q P^{t-i-1} & P^t & 0 & \cdots \\ \cdots & \sum_{\text{path}} Q^2 P^{t-2} & \sum_{i=0}^{t-1} P^i Q P^{t-i-1} & P^t & \cdots \\ & \vdots & \vdots & \vdots & \end{pmatrix} \psi(0).$$

The amplitude $\psi_n(t)$ is the coherent sum of all the amplitudes corresponding to the possible paths from $\psi_0(0)$. Note that the coin operator to reproduce the same Eq. (2) for one step is not unique. In this way, the dynamics of the FRET networks can be embedded in the Quantum Walk framework.

2 Application of Quantum Walk

One of the famous applications of Quantum Walk algorithm is search algorithm. Most of the cases are based on Grover's algorithm [3], and there are several examples including maze solving [4].

In this article, instead of considering the search algorithm application, we will introduce an application in particle physics. There is a well-studied phenomenon called "jet" which is originated by a quark production, and is well described by a parton shower algorithm [5–11] based on the Quantum Chromodynamics (QCD) theory. It is essentially a probabilistic process with the emission probabilities. Since processes in a microscopic world, such as this process observed in particle physics, are intrinsically described by quantum physics, the proper simulation requires a quantum computation or quantum simulation [12]. In particular, some properties in parton shower could be more efficiently implemented and described using the Quantum walk algorithm.

2.1 Classical Parton Shower

First, we review the parton shower algorithm to describe jets. At high-energy particle collider experiments, we expect quarks are produced. However, it is known that a bare quark is never observed because of the color confinements. Instead, due to the color charges, quark and gluon can emit a gluon, or split into quark and gluon, and we can compute the emission probability by the QCD theory. There are three types of splitting, $q \to qg$, $g \to gg$, $g \to q\bar{q}$, as depicted in Fig. 3.

It is known that the splitting probability is enhanced when the splitting occurs in a collinear way. For each step of splitting, $k \to ij$ the kinematics of the splitting is described by the 3-dimensional parameters, (θ, z, ϕ), where θ is the angle between i and j, z $(0 \le z \le 1)$ is the fraction of the momentum carried by i, that is $p_i = zp_k$, $p_j = (1-z)p_k$, and ϕ is the azimuthal angle, which is just integrable to give 2π for simplicity. The differential cross sections between the split/non-split processes, corresponding to n-final states and $(n+1)$-final states, are related as follows:

$$\mathrm{d}\sigma_{n+1} = \mathrm{d}\sigma_n \frac{\alpha_s}{2\pi} \frac{\mathrm{d}\theta}{\theta} P(z)\mathrm{d}z.$$

The QCD theory predicts the probability of the splitting with a parameter z as

$$P_{q\to qg}(z) = C_F \frac{1+(1-z)^2}{z}, \tag{3}$$

$$P_{g\to gg}(z) = C_A \left[\frac{2(1-z)}{z} + z(1-z)\right], \tag{4}$$

$$P_{g\to q\bar{q}}(z) = n_f T_R (z^2 + (1-z)^2), \tag{5}$$

where $C_F = 4/3$, $C_A = 3$, $T_R = 1/2$ based on the color algebra, and n_f is the number of the massless quark flavors.

The above expression suggests that for all cases, the enhanced region is described by $P(z) \sim 1/z$. It is known that we can assume $\theta_1 > \theta_2 > \cdots > \theta_n$ due to the interference effects; thus, having an ensemble of the events with the variety of $\{\theta\}$ is interpreted as a time evolution process by considering $1/\theta$ as time t. In this interpretation, a certain time duration Δt corresponds to $\Delta\theta$.

Following those information, once a quark exists, it will evolve based on the Poisson process with those split/non-split probabilities. At each time, splitting/non-splitting is determined by these probability functions and the final set of the tree structure is obtained, which we call a shower history. We can consider the one-to-one correspondence to the "path" of the random walk and the shower history. Note

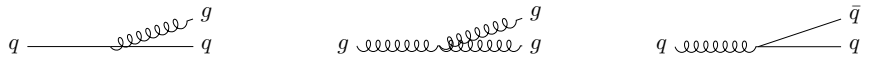

Fig. 3 QCD splitting patterns

that even for a classical parton shower algorithm, a part of the quantum interference effects is already taken into account during the computation of the splitting functions through the quantum corrections but not full.

In practice, to obtain the ensemble of the events from the parton shower algorithm, introducing the Sudakov factor is convenient, which is the non-splitting probability between the angle scale θ_i to θ,

$$\Delta(\theta_i, \theta) = \exp\left(-\frac{\alpha_s}{2\pi}\int_{\theta_i}^{\theta}\frac{\mathrm{d}\theta}{\theta}\int \mathrm{d}z\, P(z)\right). \tag{6}$$

Using the Monte Carlo method, based on the Sudakov factor, the next branching scale θ is determined by equating the random number sampled from uniform distribution $r \in [0, 1)$ as $r = \Delta(\theta_i, \theta)$. Note that $\Delta(\theta_i, \theta) \leq 1$. Alternatively, we can discretize the relevant range of the evolution between θ_i to θ_f into N steps, and introduce $\Delta\theta = (\theta_i - \theta_f)/N$. At step m, we obtain the non-splitting probability as

$$\Delta(\theta_m) = \Delta(\theta_m, \theta_{m+1}) = \exp\left(-\frac{\alpha_s}{2\pi}\frac{\Delta\theta}{\theta_m}\int \mathrm{d}z\, P(z)\right). \tag{7}$$

As long as $\Delta\theta$ is small enough, the case with more than one splitting happening at step m is negligible, therefore the splitting probability is $1 - \Delta(\theta_m)$. We need to repeat this probabilistic process N-times. Thus, it reduces to the random walk system with the probability $\Delta(\theta_m)$. With the probability we can determine the N-set of non-splitting/splitting possibilities, which provide a "path". In the end, usually an order of 10–30 partons are generated by the splitting process.

2.2 Quantum Parton Shower Algorithm

Since the splitting history can be identified as the path, we can consider the superposition of the splitting history and the interference effects. The attempt implementing this system in Quantum Walk is discussed in Ref. [13–15]. We can identify the event of non-split/split in the parton shower as the shift to the left/right in the Quantum Walk. Explicitly, the coin operator for this problem can be taken as

$$C = \begin{pmatrix} \sqrt{\Delta(\theta_m)} & -\sqrt{1-\Delta(\theta_m)} \\ \sqrt{1-\Delta(\theta_m)} & \sqrt{\Delta(\theta_m)} \end{pmatrix},$$

where $\Delta(\theta_m)$ is the non-splitting probability of a particle at step m.

We consider here a simple shower, with only one particle species that exists. The operator C is acting on the coin space $\mathcal{H}_C = \{|0\rangle, |1\rangle\}$. The $|0\rangle$ state is identified as the "no emission" state, and the $|1\rangle$ state is identified as the "emission" state. The

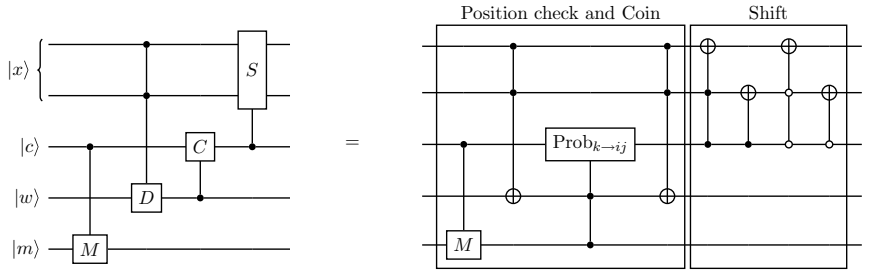

Fig. 4 Schematic quantum circuit to implement the quantum walk algorithm for parton shower. The figure is taken from Ref. [13]

position space $\mathcal{H}_P = \{|i\rangle | i \in \mathbb{N}_0\}$ represents the number of particles present in the shower and include only zero and positive integers as the parton shower cannot have a negative number of particles. The shift operation is taken as the S' in the previous section. In this way, the number of particles present in the shower is encoded in the position of the walker, with the initial state of the walker being at the $|0\rangle$ position.

It is possible to implement the Quantum Walk in the Quantum Circuit. The operator $U = S(I \otimes C)$ consists of the C acting on the coin space $\mathcal{H}_C$, which can be implemented in one qubit, and of the S, which is the conditional shift operator, which can be described by the CCNOT operator in Quantum Circuit. Figure 4 shows the schematic quantum circuit describing a single step of a quantum walk algorithm-based parton shower. In this simple shower, the number of particles present is encoded in the position of the walker, which is encoded in $|x\rangle$ in the figure. It shows a 2-qubit case, which can describe up to 4 shower particles with the initial state of the walker being at the zero position. The number of particles that the algorithm can simulate increases exponentially with the number of position qubits, x as 2^x. D describes the position check scheme, which is controlled from the position of the walker and applies the correct splitting probability accordingly in the coin operation C. The scheme is constructed from a series of CCNOT gates, thus the operation is entirely unitary. Furthermore, the position check scheme ensures that the coin operation is always applied to the $|0\rangle$ state on the coin qubit to recover the correct parton shower distribution. The subsequent shift operation then adjusts the number of particles present in the shower, depending on the outcome of the coin operation. If the coin qubit is in the $|1\rangle$ state after the coin operation, the splitting has occurred and the position of the walker is increased by one, otherwise the walker does not move. The shift operation is constructed from a series of Toffoli gates and thus is unitary. This step can be repeated for the number of discrete shower steps N in the parton shower, resembling the quantum random walk. Finally, we obtain the amplitude describing the superposition of the amplitudes with $1 - N$ shower particles. By measuring the amplitude, we can sample the "paths" with the appropriate probability.

3 Conclusion

We have reviewed the quantum walk algorithm, which can introduce the quantum interference effects to the system described by the classical random walk. From the physical setup of the FRET network, if all the quantum correlation is preserved, or the decoherence effects are negligible, the FRET network would provide a quantum device to simulate a quantum walk process. Although we need to consider the decoherence effects in a real device, it would be interesting to see what can be done in an ideal case. The real system would be modeled by the mixture of the classical random walk and the quantum walk, which would require further study. Although one of the famous applications of the quantum walk algorithm is the searching algorithm using the Grover algorithm, we have introduced an application in the parton shower algorithm in particle physics in this article. We explicitly show how to implement the quantum parton shower algorithm in the quantum walk approach. We hope a real device can help to simulate this system in future.

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