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Quantum Walk Computing: Theory, Implementation, and Application

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The classical random walk formalism plays an important role in a wide range of applications. Its quantum counterpart, the quantum walk, is proposed as an important theoretical model for quantum computing. By exploiting quantum effects such as superposition, interference, and entanglement, quantum walks and their variations have been extensively studied for achieving computing power beyond that of classical computing and have been broadly used in designing quantum algorithms for algebraic and optimization problems, graph and network analysis, and quantum Hamiltonian and biochemical process simulations. Moreover, quantum walk models have been proven capable of universal quantum computation. Unlike conventional quantum circuit models, quantum walks provide a feasible path for implementing application-specific quantum computing, particularly in the noisy intermediate-scale quantum era. Recently, remarkable progress has been achieved in implementing a wide variety of quantum walks and quantum walk applications, which demonstrates the great potential of quantum walks. In this review, we provide a thorough summary of quantum walks and quantum walk computing, including theories and characteristics, physical implementations, and applications. We also discuss the challenges facing quantum walk computing, which aims to realize a practical quantum computer in the near future.

Introduction

Quantum computing is a computing model based on quantum mechanics, and it utilizes quantum physics effects such as superposition, interference, and entanglement to achieve computational power beyond classical computing. With the great potential of quantum computing, a large number of tasks that may be intractable to classical computers can be solved with exponential or polynomial speedup by quantum algorithms. Such tasks range from factoring large prime numbers [1] and searching an unsorted database [2] to simulating quantum systems and solving large systems of linear equations. Toward the ultimate goal of building a quantum computer, enormous efforts have been made and considerable progress has been achieved. The development of quantum computing has passed through the prototype stage of demonstrating basic quantum operations and small quantum algorithms, and quantum computational advantages have also been experimentally demonstrated for certain tasks such as boson sampling [3]. While the universal fault-tolerant quantum computer remains to be built, quantum computing is now in the noisy intermediate-scale quantum (NISQ) era and possesses possibilities for tackling applications of practical interest.

The category of NISQ computers can include both analog and digital quantum devices, depending on the employed quantum computing model. There are various quantum computing models, including the quantum circuit model, quantum Hamiltonian evolution model, quantum walk model, quantum annealing model, and measurement-based quantum computation model, on which quantum algorithms and applications can be designed and implemented in quite different ways. These distinct models can hold the capability for universal quantum computing but possess different requirements for their physical implementations. Considering the properties of specific quantum computing models and the rapid progress in quantum computing hardware, quantum computing for certain applications can be achieved more quickly by exploiting appropriate models, particularly in the NISQ era.

Quantum walks (QWs) are the quantum mechanical equivalents of classical random walks. A classical random walk is used to describe a particle called a walker that moves stochastically around a discrete space, while in a quantum walk, the walker is governed by the rules of quantum physics and shows markedly distinct properties compared to its classical counterpart. Similar to the classical random walk, which forms the basis for designing many classical algorithms such as modeling share prices and describing the random movement of molecules, quantum walks have become an important model for designing quantum algorithms and also provide a promising path for implementing quantum computing [4–6]. Quantum walks have shown beyond classical potential in a variety of problems in the fields of quantum computing, quantum simulation, quantum information processing, and graph-theoretic applications, such as database search [7], distinguishing graph isomorphism (GI) [8–10], network analysis and navigation [11,12], and simulating quantum Hamiltonian dynamics [13–15]. Meanwhile, it has been proven that quantum walks on their own can implement universal quantum computing. Quantum walk models also play a key role in demonstrating quantum supremacy over classical computers, according to which a boson sampling task can be viewed as a particular instance of multi-particle quantum walk

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on specific graphs [3], and even for a single-particle quantum walk case, it has been shown that sampling quantum walk evolution probability on an exponentially large circulant graph is classically intractable [16]. Moreover, quantum walk dynamics lead to rich and complicated phenomena to be investigated [17] and present the way for exploring various features of different particles, such as multi-fermion quantum walk dynamics [18] and braiding statistics via anyonic walks [19,20].

With broad interest in quantum walks and their considerable potential, currently, a variety of quantum physical systems are used for implementing quantum walks and their applications. These physical systems include superconducting systems, trapped-ion and trapped-atom systems, bulk optics systems, and integrated photonics systems. These physical implementation approaches are rapidly developing, showing great progress in both the scalability and programmability of quantum walks. For example, experimental demonstrations of quantum walks have been realized from simple one-dimensional to high-dimensional cases and even complicated structures. The capability of controlling the parameters in the quantum walk evolution such as the evolution time, underlying Hamiltonian, and evolving particle features is continuously increasing in physical quantum walk experiments. These considerable advances in physical implementations of quantum walks allow various complicated quantum-walk-based applications and have laid a solid foundation for implementing specialized quantum walk computing systems for applications of practical interest.

Here, we present a comprehensive review of quantum walks and quantum-walk-based computing, including quantum walk models and theories, their physical implementation, and potential applications. The outline of this review is as follows: In the "Quantum Walk Theories" section, we introduce various quantum walk models, including discrete quantum walks and continuous-time quantum walks, and describe the important characteristics of quantum walks that are essential for exploring quantum walks and designing quantum algorithms beyond the classical models, and also compare these quantum walk models and discuss their relationships. In the "Quantum Walk Implementations" section, we summarize the various physical implementations of quantum walk and quantum-walk-based applications, together with the latest advancements. We provide a comprehensive overview of both the digital physical implementation of quantum walks (i.e., using quantum circuit models) and analog physical implementation of quantum walks including in solid-state, bulk optics, and integrated photonics systems. In the "Quantum Walk Applications" section, we present the advancements in the algorithms and potential applications based on quantum walk models, which comprise quantum computing applications, quantum simulation, quantum information processing, and graph-theoretic applications. Finally, in the "Conclusion and Outlook" section, we give an outlook on the future of quantum walk computing and discuss the challenges.

Quantum Walk Theories

In this section, we introduce various proposed quantum walk models, compare them, and discuss some essential quantum walk characteristics.

Quantum walks, first proposed as counterparts to classical random walks, mainly include discrete-time quantum walks (DTQWs) [21,22], which evolve step by step, and the continuous-time quantum walk (CTQW) [23–25], which evolves continuously with time. To address more complex scenarios, additional models were created, such as discrete models that can perform quantum walk evolution on directed graphs [26], nonunitary quantum walks [27] for performing evolution in an open quantum system, and discontinuous quantum walks [28,29], which combine both discrete-time and continuous-time quantum walks.

There are obvious differences between these models, but the relationships between them have also gained considerable attention in recent studies and are reflected in the transformation [30] and similar limit distributions of discrete and continuous models [31–33], the direct equivalence among different discrete models [34–36], and the generalization ability of nonunitary models for describing both quantum and classical random walks [27].

Quantum walks differ from classical random walks in terms of their evolution characteristics [23,37–41] and sampling complexity [16,42–44]. Quantum walks can accelerate the evolution process, especially for search algorithms, and have distinctive probability distributions leading to particular localization. In addition, it is confirmed to be classically hard to simulate the sampling of quantum walks such as single-particle quantum walks composed of instantaneous quantum polynomial circuits and multi-particle quantum walks, one relevant example of which is boson sampling.

Quantum walk models

Most quantum walk models can be divided into 2 types: the discrete quantum walk models and the CTQW. A discrete quantum walk has no time factor and can be realized by several steps, whereas a CTQW can be seen as a special quantum simulation within time t using a graph-related time-independent Hamiltonian. A third type of quantum walk, the discontinuous quantum walk, is composed of discrete steps of continuous quantum walks. It fuses the features of the models described above, providing a hybrid scheme for universal quantum computation. In addition to these unitary models, 2 nonunitary models are also covered here.

Discrete quantum walk models

Discrete quantum walk models incorporate a large class of models, where coin-based models and coinless models [i.e., Szegedy quantum walk (SQW) and staggered quantum walk] can be easily distinguished depending on whether there is a coin.

a. Coin-based quantum walk

The phrase "discrete-time quantum walk (DTQW)" generally refers to the coin-based quantum walk, which was first proposed as the counterpart of the classical random walk [22], as both of them are realized by 2 procedures: flipping a coin and moving in the direction determined by the flipping result. However, coin-based quantum walk requires 2 separate spaces to accomplish the above processes, namely, coin space $\mathcal{H}_C$ and shift space $\mathcal{H}_S$. In the Hilbert space $\mathcal{H}_C \otimes \mathcal{H}_S$, a quantum state $|\phi\rangle$ is defined to describe the probability amplitude of a walker arriving at a position, which can be a computational state or a superposition state where every computational state represents one position in one direction or the coin side. Owing to the superposition and entanglement of different positions, this model has a different distribution [45,46] and a quadratically faster spread [5,47] than the classical model.

We define 2 unitary transformations, namely, the coin operator $C \otimes I_S$ and the conditional shift operator S. It follows that the coin-based quantum walk can be described by a unitary

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$$U = S(C \otimes I_S). \tag{1}$$

Therefore, the state of the walker will change to $U^n \mid \phi\rangle$ from the initial state $|\phi\rangle$ after n steps [22].

The simplest example is the DTQW on a line, on which occasion the walker uses 2 coin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, to represent the 2 directions, left and right; thus, the shift operator can be defined by

$$S = |\uparrow\rangle\langle\uparrow| \otimes \sum_i |i-1\rangle\langle i| + |\downarrow\rangle\langle\downarrow \otimes \sum_i i+1\rangle\langle i|. \tag{2}$$

The choice of coin operator makes a great difference to DTQW models. Commonly selected operators include the Hadamard coin C_H and the Grover coin C_G, which are separately defined by

$$C_H = \frac{\sqrt{2}}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, C_G = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{3}$$

The DTQW on a line has interesting quantum effects [48], and more about this can be found in [48–50]. Moreover, Eq. 3 can also be extended to its N-dimensional version:

$$C_H' = \otimes_{i=1}^{\log N} H_C, \tag{4}$$

$$C_G' = \begin{bmatrix} 1-\frac{2}{N} & \frac{2}{N} & \dots & \frac{2}{N} \\ \frac{2}{N} & 1-\frac{2}{N} & \dots & \frac{2}{N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{N} & \frac{2}{N} & \dots & 1-\frac{2}{N} \end{bmatrix}. \tag{5}$$

Generally, coin-based models account for most discrete models and can be easily defined by the coin operators. For example, the Hadamard gate is used as the coin operator for the Hadamard walk [21] and a Grover coin is the coin operator of the Grover walk [51]. Table 1 also lists Lackadaisical quantum walk as a coin-based model because, although this model adds self-loops on the positions or vertices, it also contains a coin operator and a shift operator [52].

In Fig. 1, we compare the classical and quantum models on a 2-dimensional lattice and depict a path on which a walker moves from the central point to the endpoint on one diagonal of the lattice using numerical simulation. It can be seen that the classical walker can only select one path, while the quantum walker takes advantage of the coherence of all possible paths. In the quantum case, the coin operator is a 4×4 large matrix of formalism Eq. 4 and the shift operator is analogous to Eq. 2 but involves the 4 directions: up, down, left, and right.

b. Szegedy quantum walk

In 2004, inspired by the discrete-time Markov chain (time-homogeneous), Szegedy [53] proposed a quantum version with the result of faster search for the marked vertex of a graph. Subsequently, this quantum walk model, called the SQW, was adopted widely for applications relating to problems on certain graphs, such as complete graphs [54] and directed graphs [16,26].

Considering a time-homogeneous Markov chain over a period of discrete time n, the process can be expressed as $p_j(n) = \sum_i P_{ij}(n) p_i(0)$, where $p_i(t)$ is the probability of staying at the position i at time t and $P_{ij}(t)$ is the transition probability between 2 positions i and j after time t. Based on this, we can define the unitary evolution operator as a one-step coinless discrete quantum walk by determining a rule that one walker moves on an enlarged symmetric bipartite graph.

This enlarged graph should have 2 equivalent parts, A and B, both of which consist of all vertices of the original graph. If $i \in A$ and $j \in B$, then p_{ij} is the transition probability of the walker going from vertex i to vertex j, and the inverse process is expressed as q_{ij}. The evolution operator is defined as follows:

$$U = W_B W_A, \tag{6}$$

where

$$\begin{cases} W_A = 2\sum_{i \in A} |\phi_i\rangle\langle\phi_i| - I \\ W_B = 2\sum_{j \in B} |\psi_j\rangle\langle\psi_j| - I \end{cases}$$

with $|\phi_i\rangle = |i\rangle \otimes \sum_j \sqrt{p_{ij}} |j\rangle$ and $|\psi_j\rangle = \sum_i \sqrt{q_{ji}} |i\rangle \otimes |j\rangle$.

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Table 1. List of random walk models

Classical random walk models	Quantum walk models	
Discrete-time Markov chain	Coin-based DTQW	Hadamard walk [21]
		Grover walk [51,283]
		Lackadaisical quantum walk [52,284]
	Other discrete QWs	Szegedy quantum walk [53]
		Staggered quantum walk [34,35]
Continuous-time Markov chain	Continuous-time quantum walk [23]	
	Discontinuous quantum walk [28]	
	Quantum stochastic walk [27]	
	Open quantum walk [67]	

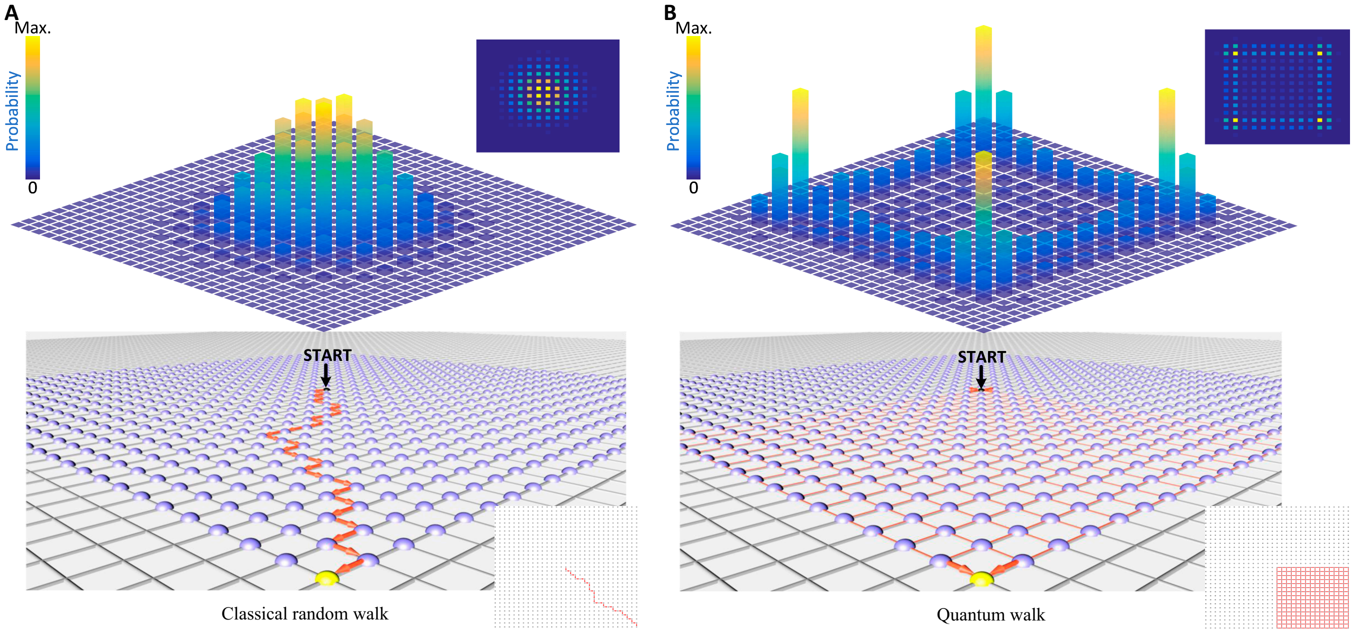

Fig. 1. Comparison of the probability distributions of the classical random walk and the quantum walk on a large lattice. The red lines depict the routes of a walker that starts from the central point and attains the yellow point after 30 steps. Above the grid is the probability distribution, which represents the possibility that the walker appears at the corresponding lattice site after 15 steps.

To clearly observe the diffusion effect of this model on the single-node state, assuming that the initial state is $|i_0, j_0\rangle$, then after W_A evolution, it is straightforward to obtain that

$$2\sqrt{p_{i_0,j_0}}\,|\,i_0\,\rangle \otimes \left(\sum_{j\neq j_0}\sqrt{p_{i,j}}|j\rangle\right) + \left(2p_{i_0,j_0}-1\right)|\,i_0\,\rangle \otimes |\,j_0\,\rangle, \tag{7}$$

where the first part indicates that the walker moves to another position with probability $p_{i_0j_0}p_{ij}$, which is the same as in the classical Markov process despite a global factor $p_{i_0j_0}$. This also implies that the SQW is a quantization of the classical random walk. Of course, if the superposition state were selected as the initialization, interference would arise between different paths, which contributes to the fact that this model performs quadratically faster than classical models in some scenarios [26,55]. A detailed description of the properties of the SQW can be found in [34, 56].

c. Staggered quantum walk

The staggered quantum walk was fully introduced by Portugal et al. [34, 35]. In this model, a graph is split into several tessellations, where any tessellation is composed of polygons, and the union of these polygons in one tessellation surrounds all of the vertices of the graph. By constructing a reflection operator associated with one of these tessellations, the walker is restricted to a one-step motion in the polygons of one tessellation, so a staggered movement, defined by the reflection operators of tessellations in several steps, can spread along all the paths in one graph [34]. The staggered model can be used for search problems if a separate reflection operator related to a partial tessellation with marked nodes is interleaved with the model. The properties of the staggered model can be studied by spectral analysis in the same manner as the Szegedy model, and particularly, the 2-tessellate case has been discussed in [36, 57]. In addition to using the reflection operators directly, considering the reflection operator as a Hamiltonian provides an alternative idea for staggered models [56,58,59] and is more friendly for the physical implementation. Recent studies have examined other properties of the staggered model, such as the spectral characteristics of the evolution operator in the 2-tessellate case [57] and robustness to decoherence and other types of noise [60].

Continuous-time quantum walk

The idea of the CTQW also originated from its classical counterpart, that is, a discrete-time Markov chain (or one-dimensional random walk) in a countable state space [23,61]. According to Kolmogorov backward equations, $\frac{dP_{ij}(t)}{dt} = \sum_{k=1}^{N} H_{ik}P_{kj}(t)$ holds for transition probability $P_{ij}(t)$ and transition rate H_{ij} to describe the jumping process that occurs instead of a diffusion process when a state i changes to the state j. For an undirected graph G of N vertices, we define

$$H_{ij} = \begin{cases} \gamma \ \text{ if vertices } i \text{ and } j \text{ are connected,} \\ 0 \ \text{ if vertices } i \text{ and } j \text{ are not connected,} \\ -\gamma d_i \ \text{ if } i = j \end{cases}, \tag{8}$$

where γ represents the hopping rate and d_i is the degree of vertex i, which is a summation of connected edges.

Let $p_i(t)$ be the probability at the position of vertex i at time t. Then, using $p_i(t) = P_{ij}(t)p_j(0)$ where $\sum_{i=1}^{N} p_i(t) = 1$ is preserved, it follows that

$$\frac{dp_i(t)}{dt} = \sum_{j=1}^{N} H_{ij}p_j(t). \tag{9}$$

For a quantum particle (or quantum walker) placed on G, a superposition state $|\psi(t)\rangle$ is used to describe its position with probability $p_j(t) = |\langle\psi(t)|j\rangle|^2$, where the orthonormal basis

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$\{|1\rangle, |2\rangle, \ldots, |N\rangle\}$ corresponds to different vertices of G. Here, imaginary unit i is introduced into the left side of Eq. 9 so that the equation can be modified to $id\,|\,\psi(t)\rangle/dt = H\,|\,\psi(\mathrm{t})\rangle$. The CTQW evolution complying with quantum mechanics is further formulated as follows

$$|\,\psi(t)\,\rangle = e^{-iHt}\,|\,\psi(0)\,\rangle, \tag{10}$$

where $H = \gamma(D - A)$ with degree matrix $D = \text{ diag }(d_1, d_2, \ldots, d_N)$ and adjacency matrix A with entries $A_{jk} = 1$ if vertices j and k are connected by an edge in G, and $A_{jk} = 0$ otherwise. The setting of the Hamiltonian H depends on what it is used for; for example, we set $H = A$ or $H = D - A$ for GI problems and use $H = |\,\omega\rangle\langle\omega\,| - A$ as a search Hamiltonian when searching for a marked vertex expressed as an oracle Hamiltonian $|\omega\rangle\langle\omega|$ [62].

It is found that the CTQW has computational speedup power over classical algorithms in some particular graphs. The first example concerns graph traversal problems known as glued-tree graphs, where Childs et al. [23] proposed a black-box quantum scheme to solve such a problem in polynomial queries, and no classical case can provide a solution in subexponential time. Other examples such as spatial search have also been proven to have a quadratic advantage [24,25] using CTQW methods, not only for searching for a marked node but also for finding several vertices in graphs.

Discontinuous quantum walk

The discontinuous quantum walk model, a fusion of the discrete-time and continuous-time models, exhibits a discrete transition from node to node via continuous-time evolution. The first discontinuous model was used to devise a scheme for implementing any universal gate [29] by way of perfect state transfers (PSTs) [28].

Every step of a discontinuous quantum walk can be considered as a CTQW, as defined in Eq. 10, namely

$$|\,v_2\,\rangle = e^{-iAt}\,|\,v_1\,\rangle, \tag{11}$$

which implements a CTQW from $|v_1\rangle$ to $|v_2\rangle$. A PST is achieved if v_1 and v_2 represent a pair of vertices in a graph. The discontinuous model makes it much easier to employ a PST between nonadjacent vertices by splitting the CTQW of an entire graph into several small-scale CTQWs on subgraphs. Subsequently, several PSTs on the vertices of well-designed subgraphs can perform a universal quantum operation [29].

Nonunitary quantum walks

Unlike the aforementioned unitary models, the following 2 models are nonunitary and act as open quantum systems. The first formalism of the nonunitary quantum walk is a continuous-time model, namely, the stochastic quantum walk. This model defines a quantum stochastic process described by density operators instead of the probability amplitudes of quantum states [27]. In the model, the Lindblad master equation is used as a general type of evolution that involves a set of axioms about all possible transition processes of connected vertices; thus, it can express random walks other than the classical Markov process and the CTQW. Nevertheless, this model may be difficult to realize experimentally in near-term quantum devices; therefore, an approach to circumvent this limitation has been proposed in [63]. Owing to its advantages in describing evolution in open systems, including both decoherence and coherence process, this model has been applied in multiple applications, such as analyzing the transport process in photosynthesis [64], PageRank [65], and function approximation, data classification, and others [66].

Analogously, there is also a type of discrete model for open quantum systems, namely, the open quantum walk model [67], which is derived directly from the formalism of the operator-sum representation. This model sparked discussions about quantum Markov processes [68–71] and studies on some of its properties such as limit distribution [72,73] and hitting time [74].

Quantum walk model comparisons

There are clear differences and relationships between the different random walks. Here, we present a detailed analysis of the difference and relationship between the original discrete-time and continuous-time quantum walk, the interchangeability of various discrete quantum walk models, including the coin-based quantum walk, SQW, and staggered quantum walk, and how nonunitary models unify the classical random walk and parts of quantum walk models.

The study of quantum walk models has progressed rapidly in recent years; however, the 2 original branches, the discrete-time and continuous-time quantum walk models, still matter in this field. No doubt there exists the obvious difference that the coin-based discrete model (DTQW) has an extra space, whereas the continuous-time model does not. Some other interesting differences must be considered. First, a DTQW requires different numbers of quantum states when performing a quantum walk on a graph. For an arbitrary graph, a DTQW introduces a quantum state for each edge of every vertex, whereas a CTQW only introduces a quantum state for each vertex. Second, it is feasible for a DTQW to regulate the coin of each step while the CTQW has to control evolution by modifying the Hamiltonian. Therefore, in the design of algorithms, an appropriate model should be selected according to the specific situation.

Despite the considerable distinctions listed above, determining the underlying relationship between these 2 models is a fundamental problem. It has been shown that they have similar spreading properties, such as faster diffusion than classical models [23,51], and the long-time limit of the DTQW with a certain coin operator is approximately equivalent to the CTQW case in terms of the probability density [31–33,75]. Moreover, in various applications, both the DTQW and CTQW algorithms work, maintaining the same performance for many algorithms, such as search [7,76] and GI [8,77], both of which can be used for universal computation [78,79]. Owing to these similarities, some studies are more concerned about how to convert between them. For example, Strauch [80] first investigated how coin-based or coinless discrete quantum walk models can be transformed into the CTQWs by taking the limit of certain parameters and blazed a path for those seeking to generalize such a transformation to higher-dimensional walks. More specific results can be seen in [30], where Childs presented a procedure for constructing an SQW to simulate the CTQW with any Hamiltonian. There is a similar theory in which the Hamiltonian of the CTQW can be discretized by the commuting adjacency matrices under the partition of a graph, where the evolution based on one adjacency matrix constitutes one step of the staggered model with Hamiltonians, which is applied to numerous graphs, such as the Cayley graph, as stated in [59]. These results demonstrate that the 2 models are interchangeable to some extent, but note that this interchangeability only means a strict approximation rather than a direct equivalence.

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However, direct interchangeability exists among various discrete models, and their relationships are shown in Fig. 2. Among discrete quantum walks, any Szegedy walk is equivalent to a 2-tessellable staggered quantum walk on the line graph of one bipartite graph [34], and both can be converted to coin-based quantum walk models on multigraphs satisfying the regularity and other conditions listed in [81]. Conversely, a coin-based quantum walk can be regarded as the SQW on a bipartite graph if the degree of vertices on one side is 2, or staggered quantum walk on the line graph if the tesselation covers the perfect matching, as in [81] and [35], respectively. More generally, any coin-based model using the flip-flop shift operator can be cast into a Szegedy model or a staggered model only if the coin operator is an orthogonal reflection despite the graph being nonregular [81]; a special example is Grover search, which can be seen as 2 steps of the Grover walk [51], a type of coined-based quantum walk with the Grover coin. Not considering strict conditions for graphs or models, a family of discrete walks regarding 2 local operators, called partition-based quantum walks [36], are unitary equivalent; that is, the evolution operators of any Szegedy model, the 2-tessellate staggered model, and the 2-step coined model are interchangeable except for a unitary multiplier [36,82].

Note that 2 models for describing walks in an open environment can cover both classical and quantum models. One is the open quantum random walk, which is a new model but also embodies existing well-known models using unitary operators, such as the Hadamard walk. With the addition of measurements after each step, the open quantum random walk can be changed into a classical model, such as a homogeneous discrete Markov chain if using well-designed Kraus operators, or a nonhomogeneous case if using general Kraus operators. For the continuous-time case, the stochastic quantum walk introduces an axiomatic formalism by means of a master equation and can not only recover a classical random walk (such as a continuous-time Markov chain) or a CTQW but also enlarge the region of continuous-time random walk models, as shown in Fig. 2.

Quantum walk characteristics

Quantum mechanic effects cause quantum walks to behave differently from classical random walks in certain properties, such as mixing time and hitting time, and allow quantum walks to handle complex problems, such as quantum sampling problems, which are difficult for classical simulation. Thus, in this section, 2 main classes of characteristics, evolution and sampling, are discussed.

Evolution characteristics

Here, we introduce some characteristics available during the evolution process of a quantum walk that have a close connection with the evolution time or probability distribution of states and are useful for demonstrating the merits of quantum models compared with classical random walks. As is shown in Fig. 1, quantum walk reveals a faster propagation and different localization compared with one of the famous classical random walk models.

• Mixing time

Mixing time is defined as a quantity for describing the shortest time when the probabilities $P(x,t)$, for different vertices where the walker stays after time t, get sufficiently close to a stationary distribution $\pi(x)$. If we define the time-averaged distribution by $\overline{P}(x,T) \equiv \frac{1}{T}\sum_{t=1}^{T} P(x,t)$, then the stationary distribution is $\pi(x) = \lim_{T\to\infty}\overline{P}(x,T)$. So, for a certain small constant $\epsilon > 0$, the mixing time [24,83] is

$$T_M^{\epsilon} = \min\left\{t \mid \left|\overline{P}(x,T) - \pi(x)\right|_1 < \epsilon\right\}, \qquad (12)$$

where $|\cdot|_1$ is the l_1 *norm*.

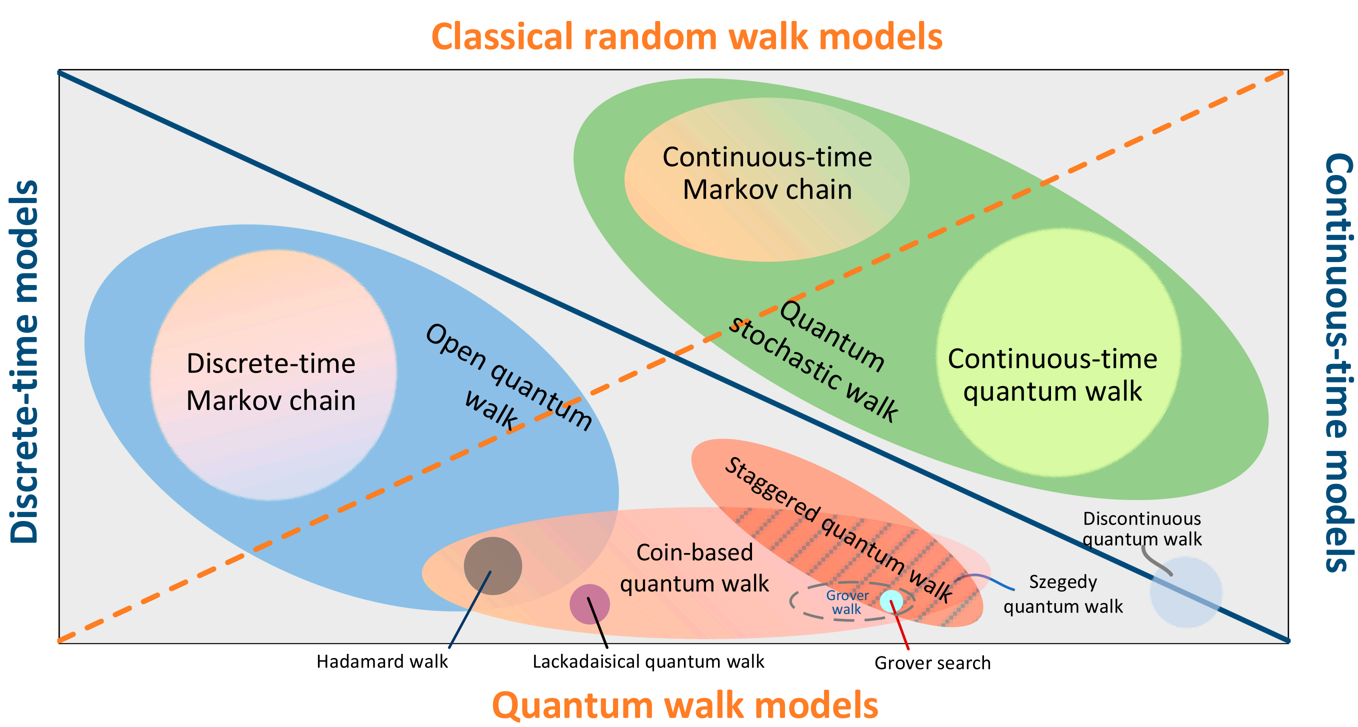

Fig. 2. Relationships between random walk models. The dashed orange line and the solid blue line are used to separate discrete and continuous models and classical and quantum models, respectively.

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Note that the mixing time for the continuous-time walk [24] shares the same definition as Eq. 12 after replacing $\overline{P}(X,t)$ with $\overline{P}(X,t) = \frac{1}{T}\int_0^T P(X,t)dt$.

• Hitting time

Hitting time is used to evaluate the time from a starting vertex to a marked vertex when detecting or searching for a target on a graph and is a vital quantity for comparing the performance of different random walks even when the exact time complexity is unknown. There are various ways to define hitting time. Generally, classical hitting time is the expected time [84] (i.e., first hitting time) at the first reaching of the end vertex, which is directly defined by

$$T_H^{ij} = \sum_{t=0}^{\infty} tP_{ij}(t), \tag{13}$$

where $P_{ij}(t)$ is the probability that the walker travels from vertex i to vertex j after time t. Analogously, the continuous version of Eq. 13 is $\lim_{T\to\infty}\int_0^T tP_{ij}(t)\,dt$.

For quantum walks, we care more about the time when the probability of hitting the target is greater than a threshold ϵ, and it has been discovered that quantum walks propagate exponentially faster than classical random walks on some graphs [23,37]. Thus, the hitting time can also be defined by

$$\tilde{T}_H^{ij} = \min\left\{t : P'_{ij}(t) > \epsilon\right\}, \tag{14}$$

where $P'_{ij}(t)$ is the probability of finding the marked vertex j from starting vertex i after time t. Another definition refers to an optimal hitting, i.e., the time related to the maximal arriving probability, which was shown to be exponentially faster than that of the classical model [38,85].

In contrast to these notions, quantum hitting time for an SQW aims to quantify the running time of searching for a marked vertex on the complete graph. Using this metric, a quadratic speedup compared to the classical algorithms was proven [84,86].

• Commute time

The term "commute time" means the expected time needed for the walker to travel from the starting vertex to the end vertex and back again. Accordingly, the commute time from vertex i to j is defined as

$$T_C^{ij} = T_H^{ij} + T_H^{ji}, \tag{15}$$

from which it is found that $T_C^{ij} = T_C^{ji}$, so the commute time is a symmetric quantity.

For a CTQW, commute time can be directly computed using the Laplacian spectrum and can help to analyze the graph-embedding property and distinguish clusters in a set of graphs [39].

• Cover time

The cover time [87] for the graph G, denoted as $\mathrm{Cover}(x, G)$ if the starting vertex is x, is the expected time to traverse every vertex. If the starting vertex is not assigned, then the cover time for an undirected graph is expressed as

$$\mathrm{Cover}(G) = \max_x \mathrm{Cover}(x, G). \tag{16}$$

This term reflects the search efficiency of a region of a graph rather than that of some specific vertex, which is the key feature that differentiates it from hitting time [88].

• Anderson localization

Anderson localization is a phenomenon of the absence of diffusion in disordered circumstances due to the interference of waves from various paths. A tight-binding model of this phenomenon [89] was first proposed by Anderson to describe the wave function (i.e., a time-independent probability amplitude) of one particle on an impure lattice. Taking the example of an electron trapped in a potential field, this phenomenon also provides a credible explanation for the metal-insulator transition [40] because the electron would be localized at a neighbor of the starting position, leading to a loss of the conductivity properties of the system, if we were to set the energy at each lattice site in a random way [90,91].

Anderson location is also an important characteristic for quantum walk models [92], where the analogous propagation impediment will arise with increases in the randomization condition, such as setting the phase-shift operator for each step [93] or randomly removing lattice sites [94]. As one of the most popular propagation models, the quantum walk also has been selected to experimentally demonstrate Anderson localization in various systems [93–96]. In contrast to the direct observation of distribution on all sites, in these experiments, more detailed qualification plays a vital part in examining the degree of the localization. For example, the average distance and number of particles on initial sites are of interest in recent related experimental studies [93,95].

Quantum dynamics and sampling complexity

In addition to their merits of evolution compared with the classical random models, quantum walks also promise quantum supremacy in terms of computing power in various scenarios, particularly for sampling problems, which have been shown to be classically intractable to simulate for both single- and multi-particle cases [16,42].

Here, we first introduce the multi-particle quantum walk, and as it is an enhanced version of the single-particle model, we set forth its capability for more complex tasks, such as simulation on a larger graph using relatively few resources by harnessing multi-particle properties. Subsequently, quantum sampling problems are briefly elaborated, and 2 examples of the single-particle quantum walk on the circulant graph and boson sampling are presented to demonstrate computational advantages beyond classical algorithms.

• Quantum dynamics of multiple particles

In contrast to distinguishable classical particles, microscopic particles at the quantum scale, like elementary particles, atoms, and molecules, are indistinguishable in principle. Indistinguishable quantum particles—whether bosons, fermions, or anyons—exhibit distinct behaviors in quantum statistics [97]. In a multi-particle system, bosons demonstrate symmetric exchange, fermion antisymmetric, while anyons, unique to 2-dimensional systems, display fractional statistics with intermediate exchange properties. So, the fact is straightforward:

$$\begin{cases} a_k^\dagger a_j^\dagger - \zeta a_j^\dagger a_k^\dagger = 0, \\ a_k a_j - \zeta a_j a_k = 0, \\ a_k a_j^\dagger - \zeta a_j^\dagger a_k = \delta_{k,j}, \end{cases}, \tag{17}$$

where a creation (annihilation) operator $a_i^\dagger\left(a_i\right)$ represents an increase (or decrease) of particle number on mode i, and ζ is set to 1, -1 or any fraction for bosons, fermions, or anyons, respectively.

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Consider any M-particle quantum walk model in Fock space, which is denoted by a unitary U without loss of generality. Its initial state can be characterized by creation or annihilation operators, and is given by

$$|\phi_{in}\rangle = \prod_i \left(a_i^\dagger\right)^{m_i} |0\rangle = \left(\prod_i m_i!\right)^{\frac{1}{2}} |M\rangle, \quad (18)$$

where $|0\rangle$ is the vacuum state and $|M\rangle = |m_1, m_2, \cdots\rangle$ is the Fock state in occupation number representation and $M = \sum_i m_i$. Specially, for m particles with a single mode, Eq. 18 can be converted to $(a^\dagger)^m |0\rangle$.

Then, after time t of evolution, the final state becomes

$$|\phi_{out}\rangle = \left(\prod_i \sum_j U_{ij}^t a_j^\dagger\right) |\phi_{in}\rangle. \quad (19)$$

Note that most problems are related to the detecting of the probability $P_{M\to T}$ of any output state $|T\rangle = |t_1, t_2, \cdots\rangle$ with initial state $|M\rangle$; thus, we formulate it as

$$P_{M\to T} = |\langle T|\phi_{out}\rangle| = \frac{\left|\sum_{\hat{\sigma}\in S_M} \zeta^{\mathrm{inv}(\hat{\sigma})} \prod_{i=1}^n \left(U_{T,M}^t\right)_{i,\hat{\sigma}(i)}\right|^2}{\prod_i t_i! \prod_j m_j!}, \quad (20)$$

where S_M is the symmetric group defined over all permutations of M elements, $U_{T,M}$ is constructed from the original unitary U by repeating the ith row t_i times and the jth column m_j times, and the function inv$(\cdot)$ represents the inversion number of one permutation.

From the fact that the dimension of Fock space grows exponentially with particle number, it becomes feasible that quantum walks on exponentially large graphs are performed using the same time as the one-particle case on a small graph [16,98–100]. To see this, consider a multi-particle CTQW on the N-dimensional Hilbert space. Its simulation scale for the one-particle CTQW will be enlarged to N^M dimensions if M particles begin walking simultaneously, which is seen from the corresponding noninteracting Hamiltonian $H(M)$ that is expressed as a direct sum of M one-particle Hamiltonians H:

$$H(M) = H^{\oplus M}, \qquad H = \sum_{ij} h_{ij} a_i a_j^\dagger. \quad (21)$$

It can be directly concluded that the multi-particle model can simulate the Cartesian product of graphs, which is a kind of N^M-dimensional graph, if all particles are distinguishable [62].

As for identical particles, the exchange symmetry between them results in a spatial dimension lower than the distinguishable case but notably higher than the one-particle case. Here are 2 examples involving bosons and fermions, both of which require a symmetrization operator $\hat{P}$ to map the Hamiltonian from Fock space to Hilbert space. We define the basis state $|\Phi\rangle = |k_1\rangle \otimes |k_2 \otimes \cdots \otimes |k_M\rangle$ on Hilbert space $\mathcal{H}^{\otimes M}$, and the symmetrization operator is described as

$$\hat{P}_{B(F)}|\Phi\rangle = \frac{1}{M!} \sum_{\hat{\sigma}\in S_M} (\zeta)^{\mathrm{inv}(\hat{\sigma})} U_\sigma |\Phi\rangle, \quad (22)$$

in which B and F represent bosons ($\zeta = 1$) and fermions ($\zeta = -1$), respectively, and $U_{\hat{\sigma}}$ is the permutation matrix associated with $\hat{\sigma}$. For fermions, if no 2 particles occupy the same vertex so that $k_1 < k_2 < \cdots < k_M$, then there are $\binom{N}{2}$ basis states, which means a reduction to the one-particle CTQW on $\binom{N}{2}$-dimensional graph. Analogously for bosons, if $k_1 \le k_2 \le \cdots \le k_M$, then it is concluded that the CTQW using multiple bosons can simulate a larger graph with $\binom{N+1}{2}$ vertices [62,99].

- The supremacy of quantum walks in sampling problems

A sampling problem is a type of problem that collects samples from a given probability distribution and acts as a solid foundation for numerous disciplines. Quantum sampling problems refer to the ones being solved by sampling (or measuring) outputs of quantum circuits, some of which are difficult to simulate using any classical algorithm; thus, they promise a demonstration of quantum supremacy in near-term quantum devices [3,43,44,101]. Sampling quantum walk evolution is similarly difficult for classical algorithms, but it could be achievable in a quantum way. Here are 2 examples.

As an important class of quantum walk models, one-particle CTQWs can be efficiently performed on graphs in the circulant class, whereas the classical simulation algorithms cannot [16], when the initial state is $|0\rangle$ and a projective measurement is applied under the basis $|0\rangle\langle 0|$. This process can be described by the following probability formulation:

$$\begin{aligned} \left|\left\langle 0|e^{-itH_c}|0\right\rangle\right|^2 &= \left|\left\langle 0|F^\dagger DF|0\right\rangle\right|^2 \\ &= \left|\left\langle 0|H^{\otimes n} DH^{\otimes n}|0\right\rangle\right|^2. \end{aligned} \quad (23)$$

This equation is easily seen to hold since the adjacency matrix H_c of any circulant graph can be factorized as a quantum Fourier transformation F and a diagonal matrix D' such that $D = e^{-itD'}$ is also a diagonal matrix. From this, a connection has been established between the CTQW and the instantaneous quantum polynomial circuits [102], which were confirmed to be classically hard to sample [43].

The same polynomial hierarchy collapse occurs in multi-particle quantum walks, as can be seen from the fact that the quantum walks of multiple bosons are equivalent to boson sampling problems in the sense of the behaviors of quantum particles. A vital step toward the classical sampling of one quantum circuit is computing probability $P_{M\to T}$ using Eq. 20. If we consider that all particles are bosons, it directly follows that

$$P_{M\to T} = \frac{\left|\mathrm{Perm}\left(U_{M,T}\right)\right|^2}{\prod_i t_i! \prod_j m_j!}, \quad (24)$$

where Perm $(\cdot)$ represents the permanent of any matrix and computing it is theoretically a #P-hard problem. Therefore, there does not exist any polynomial-time classical algorithm to simulate boson sampling [103].

Note that both of these 2 cases still hold under the condition that the classical simulation or quantum computer is noisy and imperfect, as has been confirmed based on the unproven worst-case or average-case hardness conjectures [3,103].

Quantum Walk Implementations

A variety of physical quantum systems have been used for implementing quantum walks, including superconducting

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qubits [104–106], trapped ions [107–109], nuclear magnetic resonance (NMR) [110,111], trapped atoms [112], laser beam and bulk optics [113–127], and integrated photonics systems [38,62,85,93,100,128–135]. Different quantum walk models, such as discrete-time and continuous-time quantum walks and quantum-walk-based algorithms and applications, have been experimentally demonstrated.

There are 2 different approaches to physically implementing quantum walks: analog physical simulation of quantum walks and digital physical simulation of quantum walks. In the analog physical simulations of quantum walks, the apparatus is dedicated to implementing specific instances of the Hamiltonian without translation into quantum logic, and most of the existing experimental demonstrations are of this kind. The analog physical simulation of quantum walks is not limited to graph structures, although for single-particle quantum walks it does not scale efficiently in terms of resources when simulating broad classes of large graphs. As the number of evolving particles increases, the simulated multi-particle quantum walks become classically intractable because of the exponentially large Hilbert space. The analog approach can scale by increasing the number of particles and the dimension of the Hamiltonian evolution; on the other hand, few existing methods exist for realizing error correction or providing fault tolerance in implementing analog physical simulations of quantum walks.

In digital physical simulations of quantum walks, it is necessary to construct quantum circuits for implementing quantum walk evolution. If an efficient quantum circuit can be constructed, quantum speedup can be achieved for implementing quantum walks. With such quantum circuit implementations of quantum walks, one can either implement additional quantum circuit operations or perform direct measurements of the output evolution states [16]. In general, it is difficult to design efficient quantum circuits for simulating quantum walks, although many such circuits have been found in families of graphs for different quantum walk models. However, with the digital simulation of quantum walks (i.e., quantum circuit implementations), fault tolerance and error correction in simulating quantum walks would be available by using the existing technologies in general quantum circuit computing.

We summarize in Table 2 different kinds of physical implementations of quantum walks, including both digital and analog physical implementation approaches, and compare these approaches in terms of quantum walk models, encoding methods, programmability, and scalability. Different physical implementations of quantum walks and the recent progress are further described in detail in the following sections.

Digital physical implementation of quantum walks

Quantum walk simulations in general can be implemented on a digital quantum computer, but only efficient quantum circuits promise quantum speedup compared to classical computation. Consider that if a quantum circuit that uses $O(\log(N))$ qubits and $O(\log(N))$ elementary gates can implement quantum walks on a graph of N vertices, the quantum circuit is then efficient. Efficient quantum circuit implementations for quantum walks on various kinds of graphs have been studied, as shown in Fig. 3. For DTQW models, efficient quantum circuits have been proposed for some highly symmetric graphs, including cycle, hypercycle, complete graphs, and "twisted" toroidal lattice graphs [136,137]. For non-degree-regular graphs, such as star graphs and Cayley trees with an arbitrary number of layers, quantum circuits for simulating DTQW on these graphs have also been proposed, and a quantum-walk-based search algorithm on these graphs was shown to be implemented using these circuits [138]. Loke and Wang [54] presented a general scheme to construct efficient quantum circuits for SQWs that correspond to classical Markov chains possessing transformational symmetry in the columns of the transition matrix. They further applied this scheme to construct efficient quantum circuits simulating the Szegedy walks used in the quantum PageRank algorithm for some classes of nontrivial graphs, providing a necessary tool for experimental demonstration of the quantum PageRank algorithm. This quantum circuit implementation of the SQW has been demonstrated on a programmable silicon photonic quantum processor [139].

For the CTQW model, an efficient quantum circuit implementation has been demonstrated for several classes of graphs, including commuting graphs and Cartesian products of graphs [140]. There are few classes of graphs for which the CTQWs can be fast-forwarded to obtain an efficient quantum circuit implementation. It has been pointed out that glued trees, complete graphs, complete bipartite graphs, and star graphs can be simulated efficiently using the diagonalization approach [30]. A certain class of circulant graphs have also been identified as efficiently implementable [16]. Circulant graphs can be diagonalized using the quantum Fourier transform, and by using the quantum Fourier transform circuit and inverse quantum Fourier transform circuit, a whole efficient quantum circuit for a CTQW on the circulant graph can be constructed if the given circulant graph of 2^n vertices has $O(\mathrm{poly}(n))$ nonzero eigenvalues, or has more distinct eigenvalues but can be characterized efficiently (such as the cycle graphs and Möbius ladder graphs) [16]. It is noteworthy that efficient quantum circuits for CTQWs on circulant graphs enable the simulation of circulant molecular dynamics (for example, the DNA Möbius strips) via quantum walks. Moreover, it has been proven from computational complexity theory that sampling the output probability distribution of even single-particle quantum walks on exponentially large circulant graphs could be classically intractable and thus demonstrates quantum supremacy over classical computers—this shows a new link between CTQWs and computational complexity theory. An experimental demonstration has been realized using a bulk optics quantum processor setup [16]. Also, in NMR systems, both the CTQW and DTQW using qubit models have been demonstrated [110,111]: the CTQW on a circle with 4 vertices has been experimentally demonstrated using a 2-qubit NMR quantum processor [110], and the DTQW on a square was experimentally demonstrated using a 3-qubit liquid state NMR quantum processor [111]. Among the 3 qubits, 1 qubit describes the coin state and 2 qubits describe the position state.

The digital physical simulation approach of quantum walks (i.e., quantum circuit implementation) can have the following benefits. First, quantum walks are used as a tool for designing quantum algorithms. Quantum circuit implementation can be used to efficiently implement quantum walk oracles, and further to implement the quantum walk algorithms. Second, quantum circuit implementation can provide a better estimate of the complexity and resources needed to implement quantum walk on a given graph than a "black-box" oracle. Third, to realize quantum-walk-based algorithms on a universal quantum computer, an efficient quantum circuit would be needed to implement the required quantum walk evolution.

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Table 2. Summary of physical implementations of quantum walks

	Physical systems		QW models	Encoding methods	Programmability	Scalability	References
Digital physical implementation approach	Quantum circuit implementations		CTQW, DTQW, SQW	Qubits encoded, and quantum walk evolution via quantum circuits	Full programmability through quantum circuits	Efficient circuit required for achieving speedup over classical computer	[16,30,110,111, 136,138–140]
	Solid-state quantum systems	Superconducting systems	DTQW	Each lattice site encoded into a coherent state of the cavity, and coin space into the transmon qubit	Bloch-oscillating QWs from an arbitrary split- or single-step QWs, with controllable coin operations	Scaling by increasing super-conducting qubit array	[104]
			CTQW	Each site encoded into a superconducting transmon qubit	Programmable propaga-tion paths, tunable disorders on the evolution paths, and interactions between neighboring sites, depending on the superconducting qubit array	Scaling by increasing super-conducting qubit array	[105,106]
		Trapped-ion system	DTQW	Position space encoded into the phase space and coin space encoded into 2 electronic (hyperfine) states of the ion	Controllable coin operation	Scaling up one-dimensional DTQW step number and possibly QW in higher dimension	[107–109]
		Trapped-atom system	DTQW	Coin space encoded into a 2-level particle with internal states, and position space encoded into one-dimensional spin-dependent optical lattice	Controllable coin operation	Scaling up one-dimensional DTQW step number	[112]

(Continued)

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Table 2. (Continued)

	Physical systems		QW models	Encoding methods	Programmability	Scalability	References
Analog physical implementation approaches	Optical quantum systems	Bulk optics systems	DTQW	Polarization for coin space, time-bin for position space	Controllable coin operation and initial state	Scaling up one-dimensional DTQW step number	[113–115]
				Polarization for coin space, spatial mode for position space	Controllable coin operation and initial state	Scaling up one-dimensional DTQW step number	[116–120]
				SAM for coin space, OAM for position space	Controllable coin operation and initial state	Scaling up one-dimensional DTQW step number	[121]
				Polarization for coin space, OAM for position space	Controllable coin operation	Scaling up one-dimensional DTQW step number	[122,123]
			CTQW	Quantum states are encoded in both polarization and spatial degrees of freedom	Controllable diffusion operation and initial state	Designed setup corresponding to the target quantum circuits	[124]
		Fiber systems	DTQW	Polarization for coin space, time for position space	Controllable coin operation and initial state	Scaling up one-dimensional DTQW step number	[125]
			CTQW	Site encoded in the core of multicore fiber	Quasiperiodic photonics lattices possessing both on- and off-diagonal deterministic disorder	Scaling by increasing photon and waveguide numbers	[126]
				Site encoded in supporting modes of multimode fiber	Controllable Hamiltonian configurations and initial states	Scaling by increasing the number of modes and photons	[127]
	Integrated photonics systems	Direct laser waveguide writing chips	CTQW	Spatial mode	Fixed Hamiltonian and evolution time for a given device	Scaling by increasing photon number and waveguide array size	[85,128–134]
			DTQW	Spatial mode	Fixed steps for QW for a given device, with possible particle feature control	Scaling by increasing photon number, step number and waveguide array structure complexity	[93,100]
		Silicon photonic chips	CTQW	Spatial mode	Fully programmable Hamiltonian/evolution time/particle features (using proposed entangle-ment scheme) on the same device	Scaling by increasing photon number and network size	[38,62,135]

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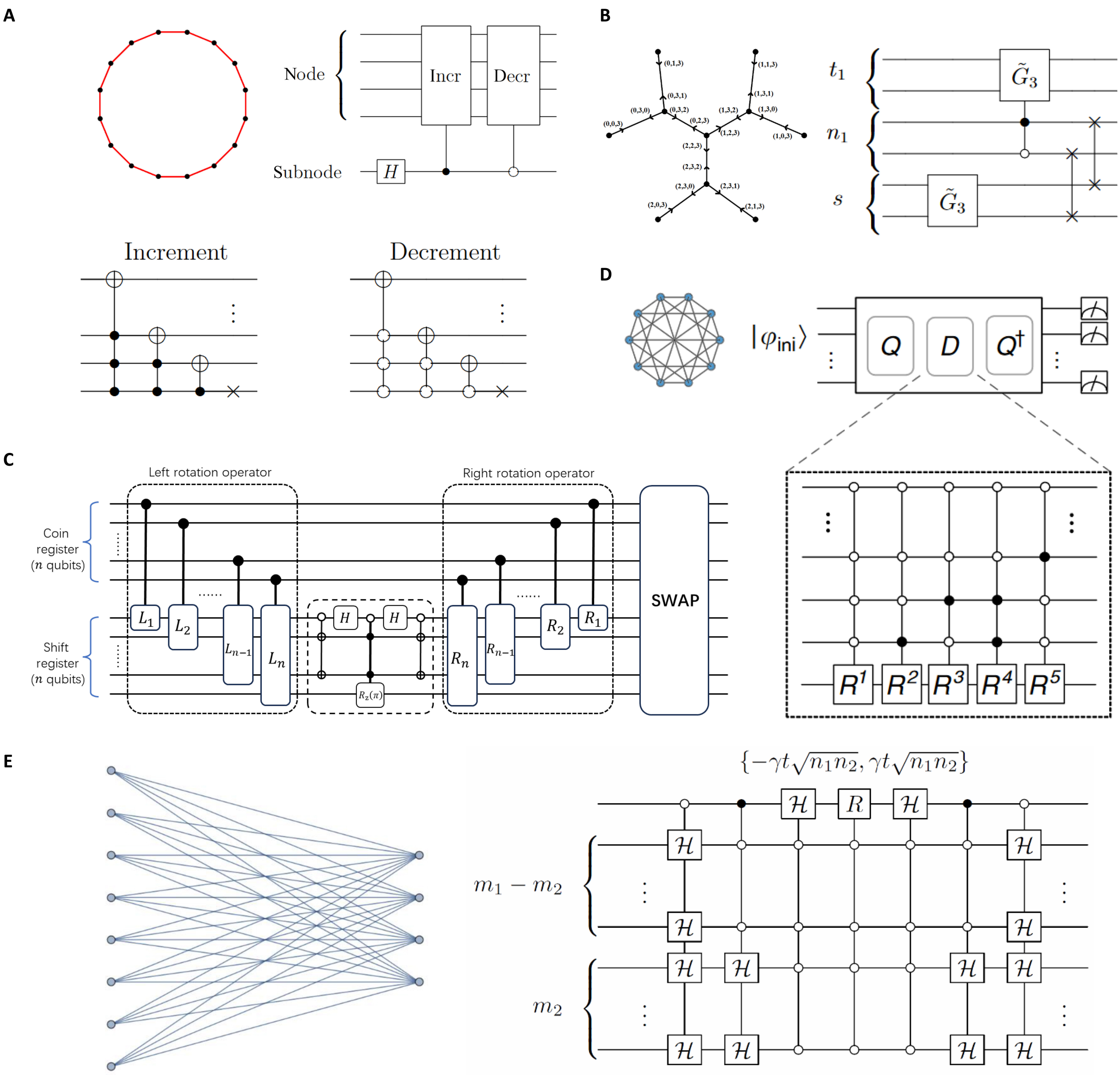

Fig. 3. Quantum circuit implementation of quantum walks. (A) Quantum circuit for implementing a DTQW on a 16-vertex circle graph. Reprinted with permission from [136]. Copyright 2009 by the American Physical Society. (B) Quantum circuit for implementing a DTQW on a 3CT-2 graph. Reprinted with permission from [138]. Copyright 2012 by the American Physical Society. (C) Quantum circuit for implementing SQWs on a cycle graph, based on [54]. (D) Quantum circuit for implementing a CTQW on a circulant graph, reproduced from [16]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (E) Quantum circuit for implementing CTQW on the complete bipartite graph [140]. Copyright 2017 IOP Publishing Ltd. Reproduced with permission. All rights reserved.

Analog physical implementation of quantum walks

The analog physical implementation of quantum walks has been demonstrated using different physical systems and has also shown great potential for accelerating useful NISQ quantum computing systems. Recently, experimental and technical advancements have been achieved in various physical systems for simulating quantum walks. Through the analog physical implementation approaches of quantum walks, a quantum-walk-based application-oriented quantum computing system is being pursued, which aims to implement different quantum walk simulations and quantum-walk-based applications. It is usually required that the quantum walk system has full programmability for quantum walk evolution. Such programmability can include (a) Hamiltonian programmability, which requires configuring the corresponding Hamiltonians of quantum walks for different instances of the problem; (b) evolution time programmability, which requires controlling the evolution time of quantum walks; (c) initial state programmability, which requires configuring the initial state of quantum walks, e.g., uniform superposition state or single basis state; and (d) particle

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feature programmability, given that particle distinguishability, particle exchange symmetry, and particle interactions can affect the output results of multi-particle quantum walks. The current analog implementation approaches to quantum walks, including solid-state, bulk optics, and integrated photonics systems, have shown the capability of these programmable abilities for various quantum walk simulations and quantum-walk-based applications.

Quantum walks in solid-state quantum systems

Quantum walks have been demonstrated using solid-state quantum systems (Fig. 4A to F), such as NMR systems, superconducting systems, trapped-ion systems, and trapped-atom systems. In NMR systems, the demonstrations of quantum walks mainly used qubit models (i.e., they used a digital physical implementation approach [110,111]), while the other systems use analog physical implementation approaches as described below.

In superconducting quantum systems, superconducting qubits can be used as artificial atoms with high-fidelity manipulation and tomographic readout, allowing them to easily simulate interacting quantum walks and explore even the hard-core boson interference in quantum walk evolution. In a circuit of quantum electrodynamic architecture, where a superconducting transmon qubit is coupled to a high-quality-factor electromagnetic cavity, considering that the quantum walk takes place in the phase space of the cavity mode, one can realize a quantum walk on a circular lattice in the cavity phase space. Ramasesh et al. [104] demonstrated that such a simulation platform associated with DTQWs is naturally suited to the direct extraction of topological invariants. Quantum walks of 1 and 2 strongly correlated microwave photons have afterward been demonstrated in a one-dimensional array of 12 superconducting qubits in the presence of strong attractive interactions [105]. Furthermore, with a 62-qubit superconducting processor, the easy programmability of the circuit enables the realization of fully configurable 2-dimensional quantum walks [106]. Experimental demonstrations show the realization of programmable quantum walks, enabling the definition of propagation paths for quantum walkers, with the remarkable control of not only the qubit frequencies but also the tunneling amplitude and phase between neighboring sites.

In trapped-ion systems, DTQWs have been demonstrated, where the simulated walker evolves along a line in a phase space [107–109]. By extending the quantum walks using 2 ions, the walker achieves the additional possibility of staying instead of taking a step [108]—the coin operation has 3 options: move left, move right, or stay. To increase the number of steps of a DTQW using a trapped-ion system, it is necessary to take into account the high-order terms of the quantum evolution. A novel protocol for quantum walks has been proposed based on a scheme from the field of quantum information processing using photon kicks [141,142] to overcome these restrictions and allow, in principle, hundreds of steps. This protocal can be extended to quantum walks in higher dimensions [109].

In trapped-atom systems, a DTQW of up to 24 steps on a line with single neutral atoms has been demonstrated, by deterministically delocalizing the atoms over the sites of a one-dimensional spin-dependent optical lattice [112]. To achieve many steps, atomic systems require formidable control and isolation from their environment, which is a challenge that must be overcome.

Quantum walks in optics systems

Optics or photon systems are currently well-developed for implementing quantum walks, among the analog implementation approaches of quantum walks. Using various methods of encoding degrees of freedom (DOFs), such as spatial modes (or path), polarization, time-bin, orbital angular momentum (OAM), and frequency, different photonic platforms have been used for implementing quantum walks (Fig. 4G to N). These photon platforms include bulk optics systems, fiber systems, and integrated photonics systems, as described in the next subsection, showing extensive techniques and promising progress in the photonic implementations of quantum walks.

In bulk optics systems, several different methods have been used for implementing DTQWs. With laser pulses as the simulated walkers, by encoding coin states in the polarizations of photons and encoding position states in the time-bin of photons, Barkhofen et al. [113] and Lorz et al. [114] successively demonstrated both 1-dimensional and 2-dimensional DTQWs with controllable coin operations. To overcome the extra loss in a conventional loop structure, Xu et al. [115] introduced birefringent crystals to implement the conditional shift operations in DTQWs, and with the polarization-encoded coin space and the time-bin-encoded position space. Alternatively, Xue et al. [116–120] used photon polarization for the coin state and the spatial mode for the position state, where the wave plates were used for coin operations and beam displacers (BDs) were used for conditional shift operations; thus, a variety of DTQWs and DTQW-based application experiments have been demonstrated.

Using the DOFs of photons, spin angular momentum (SAM) and OAM, a qubit system and a high-dimensional system can be encoded and realized, respectively, which provides a feasible method for implementing DTQWs. By encoding the coin state space in SAM and the position state space in OAM, Zhang et al. [121] used a spin-orbital system to implement a one-dimensional DTQW. Goyal et al. [122] alternatively used OAM modes as lattice sites and polarizations as the coin state to implement a DTQW with a laser beam, in a proposed ring interferometer. Giordani et al. [123] further used a similar linear optics platform for a DTQW with the OAM of photons to investigate quantum walk dynamics, demonstrating a quantum state-engineering toolbox via quantum walks. In their experiments, they used the OAM of light as the physical embodiment of the walker, while the logical states of the coin were encoded in circular polarization states.

Fiber systems are also used for implementing quantum walks, considering that bulk optical systems can have larger sizes and challenging scalability and stability. Fiber systems can easily use fiber loops to implement time-bin-encoded quantum states. Recently, some types of specialized fibers have allowed new methods of encoding quantum walks. In 2010, by encoding the coin states in the polarizations of photons and the position state in the time zone, Schreiber et al. [125] used a fiber-loop setup to implement a DTQW in 5 steps on a line with adjustable coin operations. With customized multicore ring fibers, Nguyen et al. [126] demonstrated CTQWs and localized CTQWs in a new optical fiber that has a ring of cores constructed using both periodic and quasiperiodic Fibonacci sequences. In this case, each core represents a site of CTQW and photons can be transmitted between different cores during the CTQW evolution. Furthermore, Defienne et al. [127] used a multimode fiber (MMF) to implement a quantum walk of indistinguishable

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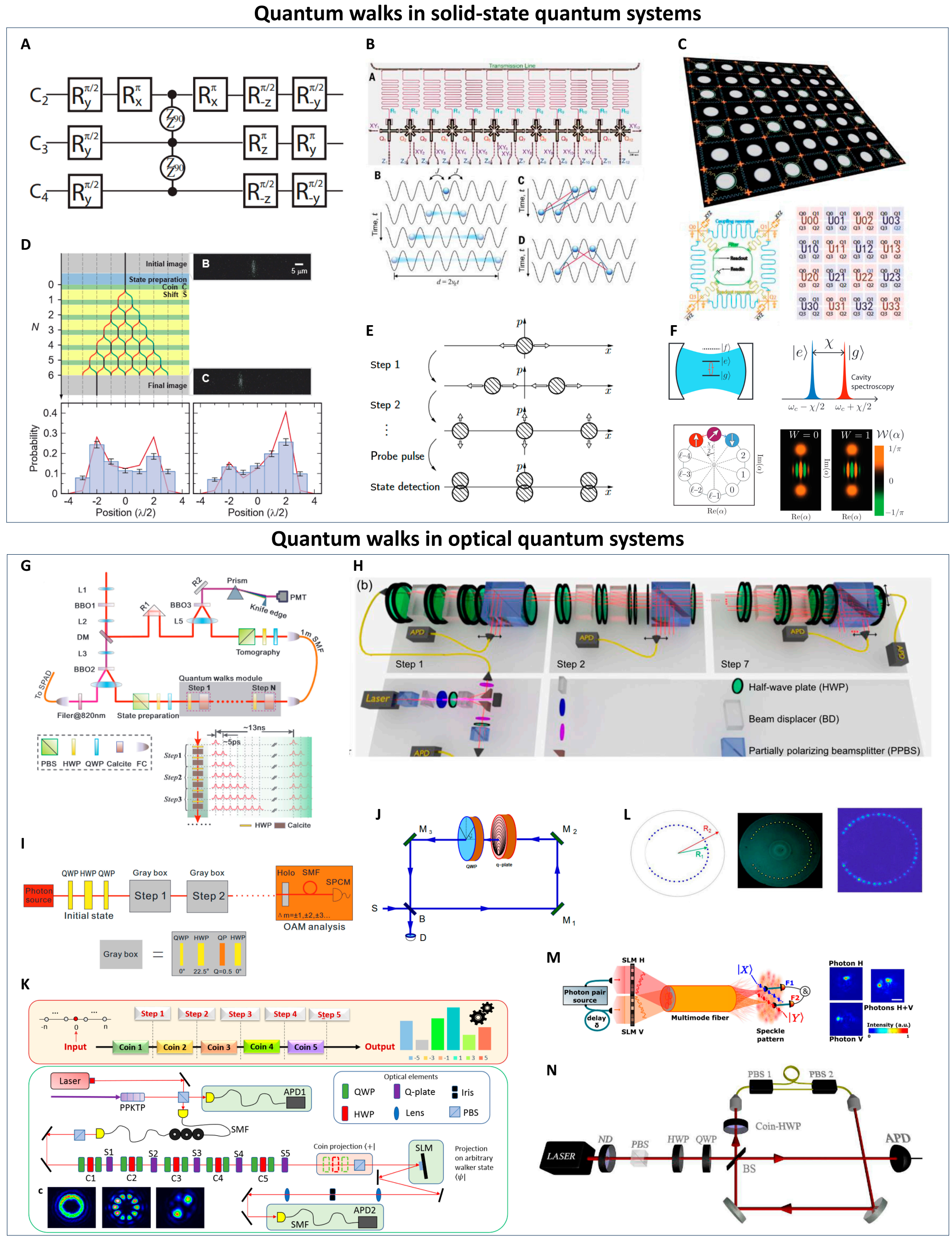

Fig. 4. Physical implementations of quantum walks in solid-state and optical quantum systems. (A) NMR pulse sequence representing a single step of DTQW. Reprinted with permission from [111]. Copyright 2005 by the American Physical Society. (B) Simulating QWs of 1 and 2 photons in a one-dimensional lattice of a superconducting processor. From [105]. Reprinted with permission from AAAS. (C) Schematic diagram of a 2D superconducting quantum processor, on which QWs on a 2D superconducting qubits array were implemented. From [106]. Reprinted with permission from AAAS. (D) 1D DTQW was implemented in position space with single optically trapped atoms. From [112]. Reprinted with permission from AAAS. (E) Schematic demonstration of a DTQW on a line in phase space using ions. Reprinted with permission from [108]. Copyright 2010 by the American Physical Society. (F) Schematic of a proposed cQED setup for realizing QWs using a superconducting cavity mode coupled to a transmon qubit. Reprinted with permission from [104]. Copyright 2017 by the American Physical Society. (G) 1D DTQW implemented in an optical system where coin space is encoded in polarization and position space is encoded in time-bin. Reprinted with permission from [115]. Copyright 2018 by the American Physical Society. (H) 1D DTQW implemented in an optical system where coin space is encoded in polarization and position space is encoded in spatial mode. Reprinted with permission from [117]. Copyright 2017 by the American Physical Society. (I) 1D DTQW implemented in an optical system where coin space is encoded in SAM and position space is encoded in OAM. Reprinted with permission from [121]. Copyright 2010 by the American Physical Society. (J) 1D DTQW implemented in the OAM space of a laser beam, where coin space is encoded in polarization and position space is encoded in OAM. Reprinted with permission from [122]. Copyright 2013 by the American Physical Society. (K) 1D DTQW implemented in an optical system where coin space is encoded in polarization and position space is encoded in OAM. Reprinted with permission from [123]. Copyright 2019 by the American Physical Society. (L) CTQW implemented in periodic and quasiperiodic Fibonacci multicore fibers, reproduced from [126]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (M) CTQW implemented in an MMF system where each site is encoded in the mode of the MMF. From [127]. Copyright The Authors, some rights reserved; exclusive licensee AAAS. Distributed under a CC BY-NC 4.0 license http://creativecommons.org/licenses/by-nc/4.0/. Reprinted with permission from AAAS. (N) DTQW implemented in a fiber optics system where coin space is encoded in polarization and position space is encoded in time-bin. Reprinted with permission from [125]. Copyright 2009 by the American Physical Society.

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photon pairs in an MMF fiber supporting 380 modes where the transmission matrix knowledge of an MMF combined with wavefront shaping methods was used, which establishes MMFs as a reconfigurable, high-dimensional platform for multi-photon quantum walks.

Quantum walks in integrated photonics systems

Integrated quantum photonics is an engineering solution proposed for the robust and fine control of photonic quantum information by allowing the generation, manipulation, and detection of photons on a single chip. It enables the miniaturization of quantum photonic experiments into chip-scale waveguide circuits, and thus provides an ideal platform for realizing devices with high subwavelength stability for generalized quantum interference experiments such as multi-photon quantum walks. By employing photons as quantum walkers on intrinsically stable integrated waveguide arrays that are used as quantum walk evolution networks, integrated photonics devices have been extensively used for implementing multi-particle quantum walks on large networks with even more complicated structures (Fig. 5A to F). In some integrated photonics devices, each waveguide is generally coupled to several other waveguides, enabling the fabrication of structures that are directly mapped to graphs with a high degree of connectivity with different coupling strengths for nearest and non-nearest neighboring waveguides. In this way, it is equivalent to the adjacency matrix of the graph that represents the waveguide structure on which the CTQW evolves. In addition, a reconfigurable on-chip optical network, consisting of Mach–Zehnder interferometers (MZIs) and phase shifters, can be programmed into an arbitrary optical unitary transformation [143] and is thus used for implementing the quantum walk evolution with different Hamiltonians by reconfiguring the on-chip network easily (Fig. 5G and H).

In 2010, Peruzzo et al. [128] first demonstrated a one-dimensional CTQW in an array of 21 continuously evanescently coupled waveguides in a SiOxNy (silicon oxynitride) chip, and they simulated one-particle walking on a 2-dimensional lattice by injecting 2 indistinguishable photons into the chip. With the technology of direct laser waveguide writing, waveguide chips have been fabricated for 1-dimensional to 2-dimensional quantum walks and for quantum walks with complicated structures. In 2014, Poulios et al. [129] demonstrated the quantum walks on an integrated photonic waveguide chip with a 2-dimensional "Swiss cross" structure and implemented quantum walks on a more complex graph structure of 45 vertices and 126 links by performing quantum walks of 2 indistinguishable photons in the "Swiss cross" waveguides. In 2021, Benedetti et al. [130] demonstrated the CTQW evolution in a planar triangular lattice structure waveguide chip on a fused-silica substrate fabricated using the femtosecond-laser writing technique and implemented a CTQW-based spatial search on 2-dimensional triangular graphs. With a maze of tens of waveguide modes fabricated by femtosecond-laser waveguide writing, Crespi et al. [131] demonstrated that a quantum walker traveling in a maze can achieve extremely efficient and fast transmission.

Both the scalability and complexity of the waveguide structure fabricated by femtosecond-laser writing techniques have achieved rapid developments in recent years, and different quantum walk evolution dynamics have been demonstrated. With a 2-dimensional structure of waveguides up to 160 modes, Jin et al. [85] experimentally demonstrated quantum fast hitting on hexagonal graphs, achieving a linear relationship between the optimal hitting time of CTQW and the network depth. By using a waveguide chip containing nearly 700 sites, they further implemented CTQWs in fractal photonic lattices and experimentally investigated quantum transport in fractal networks, which further revealed the transport process through either the direct observation of photon evolution patterns or the quantitative characterization [132]. By using femtosecond-laser direct writing techniques, various large-scale structures that form a 2-dimensional lattice with up to 37×37 and 49×49 sites have been implemented on photonic chips [133,134]. These chips can be used to simulate much larger graph structures by using an injected 2-photon state; for example, using a chip of 37×37 sites, Jiao et al. [133] simulated a single-photon CTQW in a higher dimensional graph structure that contains 1,369 sites and 6,600 edges.

Although the femtosecond-laser writing technique is mostly used for fabricating waveguide chips for implementing CTQWs, it also provides a good platform for implementing DTQWs. With a disordered lattice realized by an integrated array of interferometers fabricated in glass by femtosecond-laser writing, Crespi et al. [93] experimentally implemented the DTQW with 8 steps and observed the Anderson localization of entangled photons in a DTQW affected by position-dependent disorder. With a femtosecond-laser-written waveguide chip, Sansoni et al. [100] implemented an array of beam splitters for a 4-step quantum walk and experimentally demonstrated how particle statistics, either bosonic or fermionic, influence a 2-particle DTQW.

Silicon quantum photonics, taking advantage of its high component density, full programmability, and CMOS (complementary metal oxide semiconductor) compatibility, has become a very promising approach for implementing large-scale photonic quantum computing [62,139,144–146] and universal quantum computing [147]. With well-developed on-chip photonic quantum state generation and manipulation, silicon quantum photonics also presents an ideal platform for implementing quantum walk simulations and quantum-walk-based algorithms. Silicon photonics can implement on-chip reconfigurable linear optical networks consisting of MZIs and phase shifters that are universal for arbitrary unitary operations. With such reconfigurable on-chip networks, quantum walk evolution on arbitrary graph structures can be implemented, and with multiple photons injected into the network, multi-photon quantum walks can be performed. In addition, with control over entangled photons and reconfigurable optical networks on chip, the full programmability over quantum walks, such as Hamiltonian programmability, evolution time programmability, initial state programmability, and particle feature programmability, has been studied [100,148] and experimentally demonstrated in silicon quantum photonics [38,62,135].

In 2021, Qiang et al. [62] first implemented a universal multi-particle quantum walk processor in silicon quantum photonics by exploiting an entanglement-driven scheme, and they realized quantum walks with full control over various parameters in one device, including the evolution time, initial state, underlying graph structures, particle exchange symmetry, and particle indistinguishability. The device can implement 2-photon quantum walks on any 5-vertex graph with continuously tunable particle exchange symmetry and indistinguishability. Using the device, they showed how this simulates single-particle walks on larger graphs, with the size and geometry controlled by tuning

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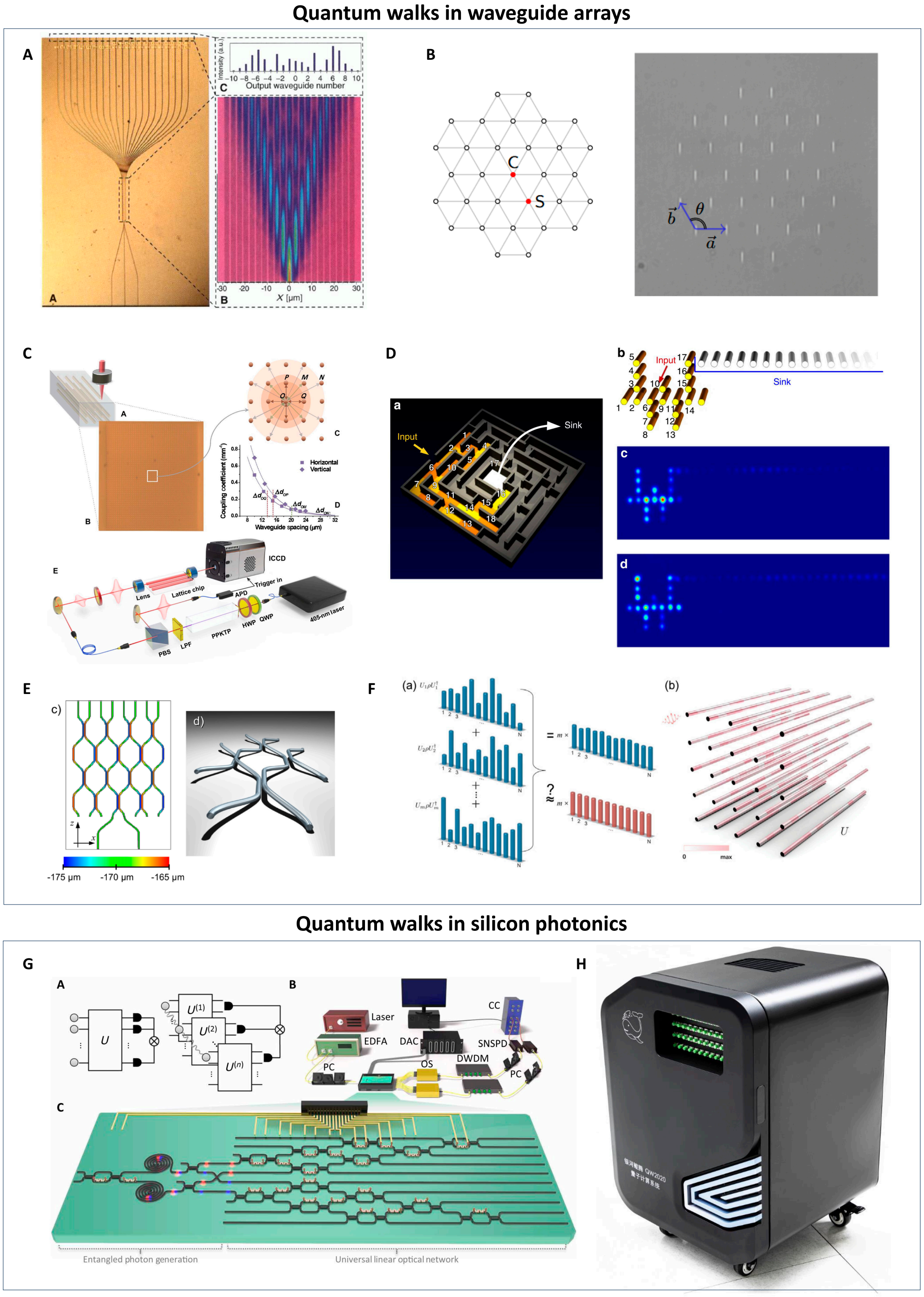

Fig. 5. Physical implementations of quantum walks in integrated quantum photonics devices. (A) A continuously coupled waveguide array in a SiOxNy chip for implementing CTQWs of correlated photons. From [128]. Reprinted with permission from AAAS. (B) CTQW-based search demonstrated in a 2-dimensional array of optical waveguides fabricated by the femtosecond-laser direct writing techniques. Reprinted with permission from [130]. Copyright 2021 by the American Physical Society. (C) A 2-dimensional waveguide array for CTQWs on lattices up to 49 × 49 nodes fabricated using femtosecond-laser direct writing techniques. From [134]. Copyright The Authors, some rights reserved; exclusive licensee AAAS. Distributed under a CC BY-NC 4.0 license http://creativecommons.org/licenses/by-nc/4.0/. Reprinted with permission from AAAS. (D) A 2-dimensional integrated waveguide array for stochastic quantum walk on a maze, reproduced from [279]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (E) An integrated optical circuit consisting of waveguides and directional couplers fabricated using femtosecond-laser direct writing techniques, and it implements a 4-step DTQW. Reprinted with permission from [100]. Copyright 2012 by the American Physical Society. (F) Illustration of 2-dimensional stochastic quantum walks on the integrated photonic chip used for generating Haar-uniform randomness. Reprinted with permission from [280]. Copyright 2022 by the American Physical Society. (G) A programmable silicon quantum photonic processor for implementing CTQW with full control over various QW evolution parameters in one device. From [62]. Copyright The Authors, some rights reserved; exclusive licensee AAAS. Distributed under a CC BY-NC 4.0 license http://creativecommons.org/licenses/by-nc/4.0/. Reprinted with permission from AAAS. (H) A system with the core of fully programmable silicon quantum photonics chip for implementing large-scale quantum walks, reproduced from [38]. Distributed under a CC BY-NC 4.0 license http://creativecommons.org/licenses/by-nc/4.0/.

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the properties of the composite quantum walks. Employing such full programmability, different quantum-walk-based algorithms were experimentally demonstrated using the device, such as searching for vertices in graphs and testing for GI. The increasing integration scale of silicon quantum photonics enables a larger scale of quantum walk simulations. Using the same protocol for universal multi-particle quantum walk simulation, Wang et al. [38] further implemented larger-scale quantum walks using a fully programmable large-scale silicon photonic quantum walk processor, which enabled the simulation of quantum walk dynamics on graphs with up to 400 vertices. With this system, they demonstrated the exponentially faster hitting and quadratically faster mixing performance of quantum walks over classical random walks, achieving more than 2 orders of magnitude of enhancement in the experimental hitting efficiency and a reduction of almost half in the experimental evolution time for mixing. They implemented numerous large-scale quantum-walk-based applications, including measuring the vertex centrality and searching for marked vertices in networks of up to hundreds of nodes. Moreover, such full programmability over quantum walks by using silicon quantum photonics provides methods for simulating other physics via the dynamic behavior of quantum walk evolution; for example, the topological phase of higher-order topological insulators can be simulated in the same quantum walk processor [38], and by implementing a time-reversal symmetry-breaking quantum walk on a reconfigurable silicon photonic device, the enhancement introduced by breaking time-reversal symmetry was experimentally demonstrated [135].

Quantum Walk Applications

Along with the excellent development of quantum walk theories and rapid progress of quantum walk implementation techniques, the exploration of quantum walk applications has flourished. We divide quantum walk applications into 4 main categories: quantum computing, quantum simulation, quantum information processing, and graph-theoretic applications, as shown in Fig. 6. These 4 categories represent the different aspects of exploiting the potential of quantum walks. First, as the quantum counterpart of the well-known classical random walk, quantum walks are naturally assumed to be capable of designing quantum-walk-based algorithms that may outperform their classical counterparts in a broad class of applications. Considering their capability for universal quantum computation, quantum walk models provide a sufficient possibility for designing quantum algorithms. Second, quantum walk evolution describes the physical process of quantum particle evolution and presents a method for solving quantum simulation applications via quantum walks. Quantum walk on its own provides a framework for studying multi-particle properties, for example, bosonic, fermionic, and anyonic particle characteristics; moreover, it can act as a general approach for simulating Hamiltonian dynamics and in applications of molecular analysis and biochemical processes. Third, quantum walks can serve as a comprehensive toolbox in the field of quantum information processing for the preparation, manipulation, characterization, and transmission of quantum states, and this paves the way for the development of new techniques for quantum information processing applications, for example, applications based on quantum walks, novel protocols for quantum communications, and new algorithms for quantum cryptography have been proposed. Finally, because the underlying Hamiltonian that determines the evolution of quantum walks is directly associated with the structure of a graph, quantum walks are a promising tool for solving graph-theoretic applications such as exploring the structure of a graph more efficiently or distinguishing between graph structures more precisely. Thus, a variety of network applications can be addressed using quantum walks by mapping them to related graph-theoretic problems.

Quantum computing

A critical part of quantum computation is to design appropriate quantum algorithms for different problems, which is quite a challenging task. In the commonly used quantum circuit model, a quantum circuit acts on a fixed number of qubits and terminates with a measurement. Similarly, quantum walk models provide a new approach to designing quantum computing algorithms (Fig. 7A and B): a particular quantum walk evolution with an input initial state is performed, and the probability distribution of the output evolution state is usually sampled to extract results. Quantum walk models are a versatile tool in quantum computation; they are proven to be universal for quantum computation, and thus, any other quantum algorithms in theory can be implemented via quantum walks; furthermore, quantum walks are the quantum counterparts of the well-known classical random walks, and thus, they open up a new avenue for designing quantum walk algorithms that can outperform classical random walk algorithms.

Quantum walks have been shown to be capable of performing universal quantum computation. The power of the quantum walk as a universal model of quantum computation was first explored by Childs [78] in 2009, when he demonstrated that a CTQW can be used for universal computation in the sense that any quantum computation can be simulated by a quantum walk on a sparse, unweighted graph of low degree. Subsequently, Childs et al. considered multi-particle quantum walks with interactions and showed that any n-qubit circuit with g gates can be simulated by the dynamics of $O(n)$ particles that interact for time $\mathrm{poly}(n, g)$ on a weighted planar graph of maximum degree 4 with $\mathrm{poly}(n, g)$ vertices, which means that a multi-particle quantum walk is capable of performing efficient universal quantum computation [6]. In 2010, Lovett et al. showed that a DTQW is also capable of universal quantum computation, and thus can be regarded as a computational primitive similar to a CTQW [79]. Underwood and Feder [29] extended this concept to discontinuous quantum walk, in which a quantum walker takes discrete steps of CTQW evolution, and showed that it is also a universal model of quantum computation. These studies have collectively shown that quantum walk models are capable of universal quantum computation, which may inspire a new architecture of a quantum computer that does not require complex control and also provide tools for designing quantum algorithms and analyzing quantum computation theory. To explore the full power of universal quantum-walk-based computation, recent studies on error correction in quantum walk evolution may be important in this field [149,150]. For example, based on the 2-lattice Bose–Hubbard model, a quantum walk error correction algorithm can reduce the decoding time of the error correction process and achieve a high fault-tolerance rate [150]. In addition, some error mitigation strategies are useful for reducing the impact of noise on particles during quantum walks [151,152].

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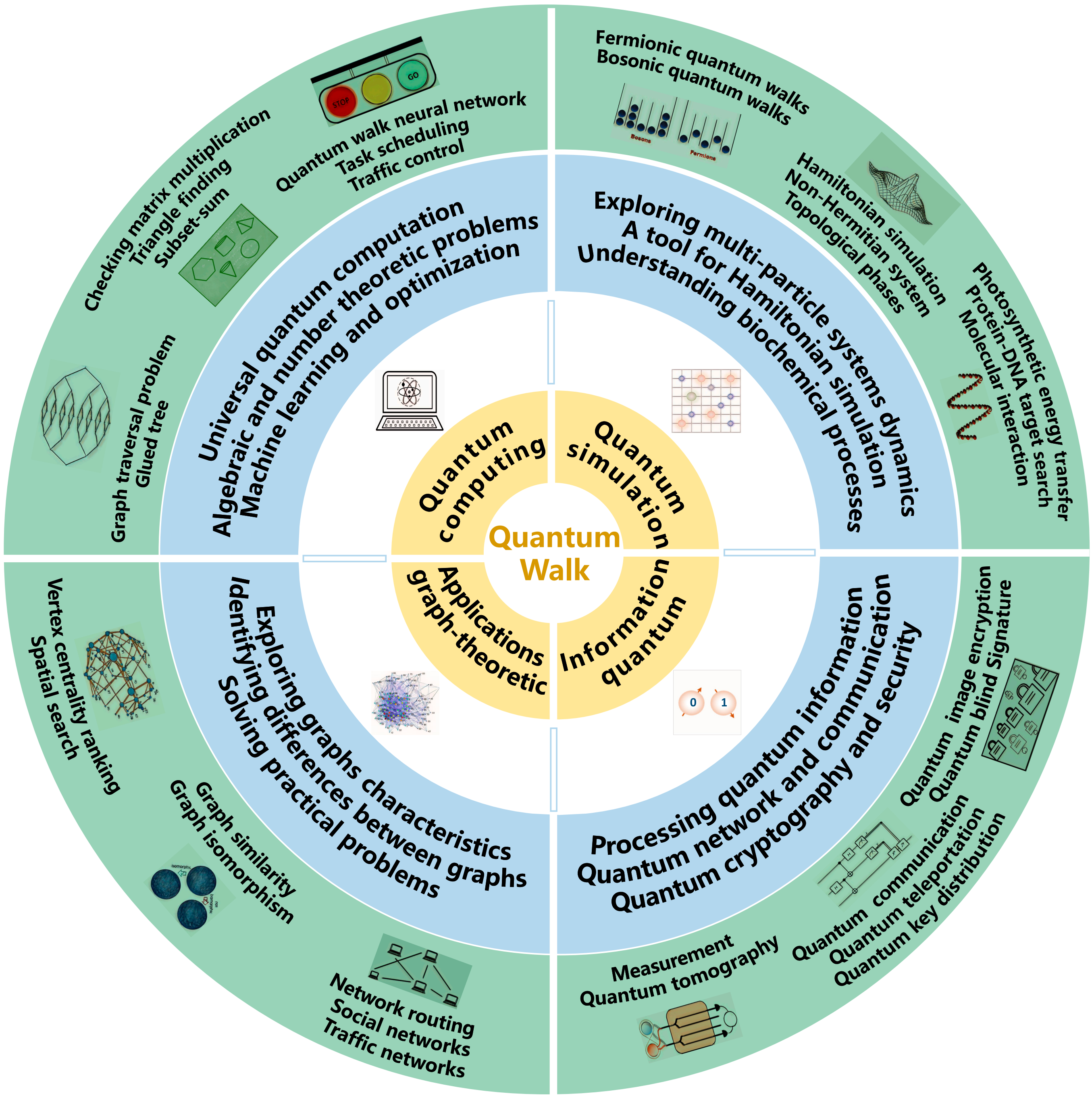

Fig. 6. Summary of quantum walk applications. They are divided into 4 main categories: quantum computing, quantum simulation, quantum information processing, and graph-theoretic applications.

Quantum walks have been widely used in designing quantum algorithms that can achieve computational speedup over classical algorithms for various problems, particularly algebraic and number-theoretic problems. Typically, for black-box problems, quantum walk algorithms can achieve exponential speedups. A well-known example is the glued-tree problem [23]: a glued tree is a graph obtained by taking 2 binary trees of equal height and connecting each leaf of one tree to exactly 2 leaves of the other tree such that the degree of each node that was a leaf in one of the original trees is now exactly 3. It has been shown that the time taken by a CTQW on this glued tree to reach the right root from the left one is exponentially faster than the classical random walk [23], and a proof-of-principle experimental demonstration was also presented [153]. Another example is a quantum algorithm for finding hidden nonlinear structures over finite fields [154]. The algorithm is based on a quantum walk on a graph that encodes the structure of the black-box function. An exponential speedup arises from the quantum interference effect, which allows the quantum walker to explore the search space more efficiently than classical algorithms.

For some algebraic problems, quantum walks have the potential to achieve a polynomial computational speedup over classical

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algorithms, leading to faster and more efficient solutions. For example, Ambainis [155] presented an optimal quantum algorithm for the element distinctness problem, where for determining whether all elements of a list of size N are distinct, only $\Theta(N^{2/3})$ queries are required using a quantum walk algorithm, whereas classically $\Omega(N)$ queries are required. In the problem of formula evaluation, a formula is encoded into a tree with a gate at each internal node and an input bit at each leaf node, and the task is to evaluate the output of the root node when given oracle access to the input. With a quantum-walk-based algorithm, the formula evaluation problem can be solved using many fewer queries, achieving a polynomial speedup compared to classical algorithms [156]. In addition, quantum walks have been applied to other problems in algebraic theory and number theory, such as checking matrix multiplication [157], testing group commutativity [158], subset sum [159], and triangle finding [160]. These quantum walk algebraic algorithms have important implications for applications in various fields, including cryptography, data analysis, drug discovery, and optimization, and can serve as the basis for designing other quantum computing algorithms or protocols.

Quantum walk models have also been investigated in the fields of machine learning and optimization and show promise for the design of quantum neural networks with new structures and algorithms. For example, Dernbach et al. proposed a quantum walk neural network [161], where the neural network architecture learns a quantum walk on a graph by learning the coin operator and then uses this learned quantum walk to form a diffusion operator to act on the input data. They obtained competitive results compared to other graph neural network approaches. Schuld et al. studied the use of quantum walks as an approach to quantum neural networks, using the formalism of quantum walks to determine the dynamic evolution of a quantum neural network that optimizes the computational properties of classical neural networks [162]. Quantum walks have also been explored to enhance classical neural networks, for example, during the training of a classical artificial neural network, where a quantum walk algorithm is applied to search for weights [163]. For addressing usually NP-hard optimization problems, a quantum walk optimization algorithm was developed by Marsh and Wang [164,165]. It utilizes an efficient indexing algorithm in conjunction with a generalization of the quantum approximate optimization algorithm mixing operator to a CTQW over a circulant graph that connects all feasible solutions. The algorithm was applied to the NP-hard problem of portfolio optimization with discrete asset constraints to find high-quality solutions to the portfolio optimization problem [166] and demonstrated the applicability of the quantum walk optimization algorithm to the capacitated vehicle routing problem [167], where the algorithm achieved the expected qualities with less computational effort than is required by classical random sampling. Other optimization algorithms based on quantum walks have also been proposed, such as a clustering algorithm based on one-dimensional quantum random walks that were applied in network cluster server traffic control and task scheduling [168] and the quantum backtracking algorithm proposed by Montanaro [169], which consists of solving a constraint satisfaction problem by constructing a backtracking tree and exploring it using a quantum walk.

Quantum simulation

Quantum simulation uses a controllable quantum system to simulate the behavior of other quantum systems. It aims to gain insight into complex quantum phenomena that are difficult or impossible to analyze using classical computers. This is a rapidly growing field, ranging from molecules and materials to quantum field theories. Quantum walks can be used as tools for quantum simulation (Fig. 7C to F) and have potential applications in simulating multi-particle systems, solving complex physical problems, and understanding biochemical processes. By using quantum walks to simulate these systems, one can gain in-depth knowledge of their properties and behavior.

Quantum walk evolution provides a path for exploring multi-particle quantum dynamics and various characteristics. The applications of multi-particle quantum walks depend on various factors, including the number, exchange symmetry, and indistinguishability of the particles involved, and the underlying graph structures in which they move. Furthermore, entangled photons can be used to simulate multi-particle quantum walks with bosonic, fermionic, or anyonic statistics using an entanglement-based scheme. This method was first used in [100,148], where both a CTQW and DTQW of 2 particles were experimentally demonstrated. Specifically, Sansoni et al. [100] demonstrated the implementation of a 2-particle bosonic-fermionic quantum walk using integrated photonics. Matthews et al. demonstrated the simulation of fermionic statistics with photons in one-dimensional CTQW evolution [148]. These experiments show that differences in particle exchange symmetry can affect the quantum walk dynamics owing to the Pauli exclusion principle (Fermi–Dirac statistics) or Bose–Einstein statistics. Using an extended entanglement-based protocol, Qiang et al. [62] demonstrated the CTQW evolution of multiple particles with both tunable particle exchange symmetry and indistinguishability by adding control over the entangled photons. In 2022, Wang et al. [38] realized a large-scale fully programmable quantum walk and demonstrated the use of this platform to simulate the behavior of multi-particle systems and explore topological phases in quantum systems using quantum walks, including higher-order topological insulators. In addition, a larger quantum walk can be used to simulate the behavior of multi-particle quantum walks on a smaller graph to investigate multiple-particle dynamics. In 2012, Schreiber et al. [170] demonstrated the use of a 2-dimensional quantum walk on a larger graph to simulate the dynamics of 2 interacting particles on a one-dimensional graph.

A quantum walk can act as a general approach for simulating quantum Hamiltonian dynamics and investigating their various properties. Berry et al. proposed algorithms for simulating nonsparse Hamiltonians with nearly optimal dependence on all parameters by implementing a combination of quantum walk steps with fractional-query simulation [171]. They also proposed an algorithm for simulating Hamiltonians using a black-box approach [15], where the Hamiltonian is treated as an oracle. These algorithms aim to improve the efficiency of Hamiltonian simulation, particularly for nonsparse Hamiltonians. Berry and Novo [172] proposed a method to simulate Hamiltonian evolution by repeatedly using a superposition of the steps of a quantum walk and then applying a correction to the weightings for the number of steps of the quantum walk. In conventional quantum mechanics, the Hamiltonian describing a quantum system must be Hermitian, and the corresponding evolution is a unitary process. However, in practice, physical quantum systems are typically open, which means that they interact with their environments and exchange energy and information with them, resulting in non-Hermitian systems. One approach to

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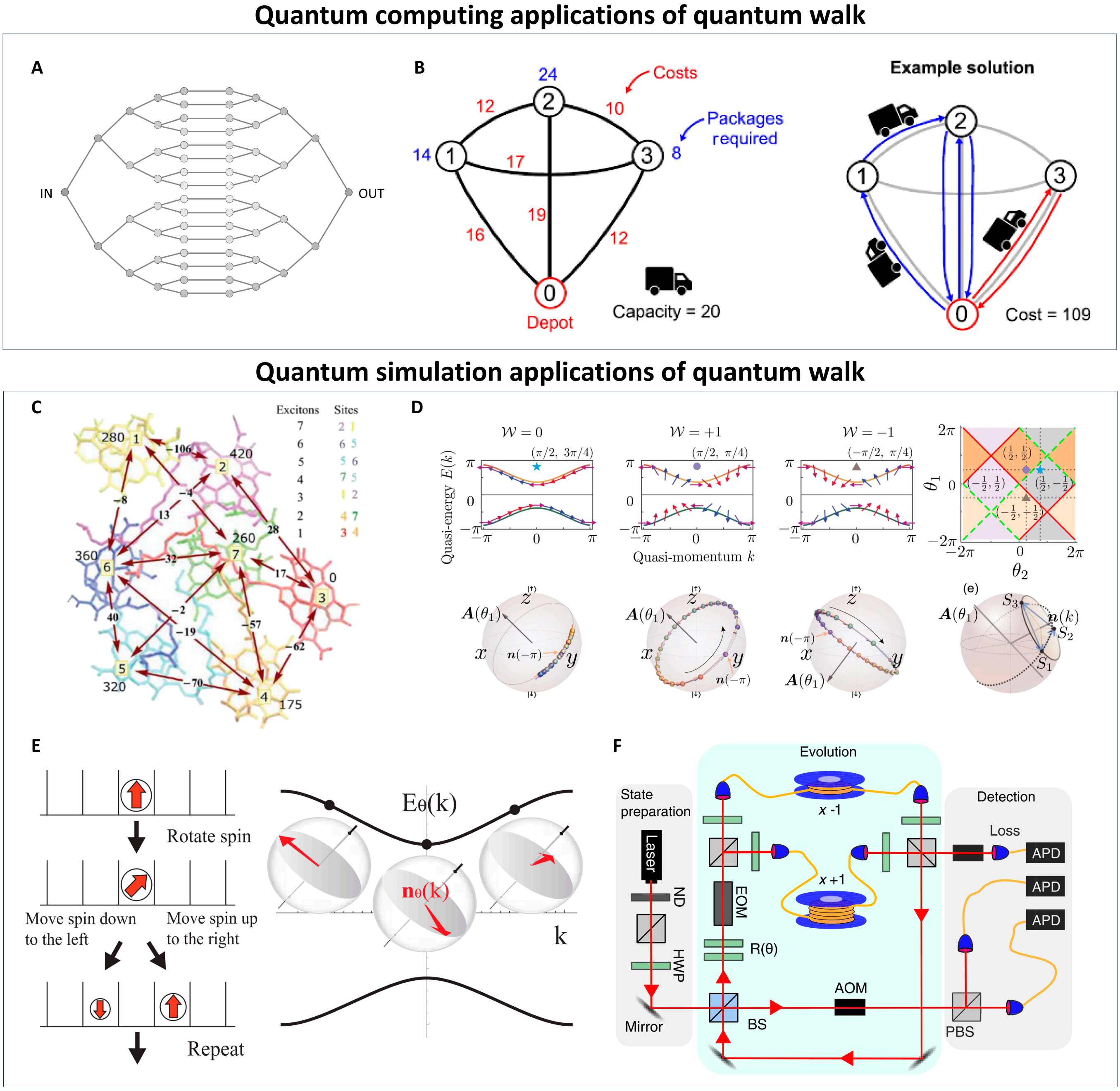

Fig. 7. Quantum computing and quantum simulation applications of quantum walks. (A) Schematic diagram of the glued-tree problem for which a CTQW achieves exponential speedup over classical random walk, based on [23]. (B) Example of a capacitated vehicle routing problem of size $n = 3$ with vehicle capacity $V = 20$. Reprinted from [167]. Copyright 2021 Bennett, Matwiejew, Marsh, and Wang. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (C) Structure of the Fenna–Matthews–Olson protein. Quantum walks can enhance the excitation energy transfer for the Fenna–Matthews–Olson protein complex. Reprinted with permission from [14]. Copyright 2008 by the American Physical Society. (D) Topological properties of a split-step DTQW in the standard time frame. Reprinted with permission from [115]. Copyright 2018 by the American Physical Society. (E) The realization of one-dimensional topological phases in DTQWs. Reprinted with permission from [281]. Copyright 2010 by the American Physical Society. (F) Time-multiplexed implementation of the photonic quantum walk to simulate non-Hermitian quasicrystals. Reprinted with permission from [173]. Copyright 2022 by the American Physical Society.

simulating non-Hermitian systems using quantum walks is to introduce a complex potential into the walk [173–175], which breaks the symmetry of the system and allows for the simulation of non-Hermitian behavior. Another approach is to implement a nonunitary quantum walk [176,177], which allows the simulation of non-Hermitian systems without requiring the introduction of a complex potential. Parity-time (PT) symmetric systems are a special type of non-Hermitian systems in which the eigenenergies of the PT-symmetric non-Hermitian Hamiltonian are entirely real. In 2017, Xiao et al. [119] proposed a quantum walk model suitable for PT-symmetric systems and experimentally realized PT-symmetric DTQWs with single photons. Quantum walks can also be used to explore quantum thermodynamic behavior. Romanelli et al. [178,179] investigated the

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thermodynamic behavior of a DTQW on a line and extended it to N-dimensional systems. They also explored the relationships between quantum walks, entanglement, and the laws of thermodynamics, demonstrating that entanglement plays a key role in the thermodynamic behavior of quantum walk models [180]. Wang et al. [181] experimentally verified the generalized eigenstate thermalization hypothesis and generalized thermalization in a photonic DTQW.

Topological phases exhibit unique properties that challenge our understanding of phases and phase transitions. Instead of being characterized by local order parameters, these phases are defined by nonlocal topological invariants that determine the existence and number of topological edge states at the interface between the bulk and boundary regions through what is known as the bulk-boundary correspondence. Quantum walks provide new insight into the simulation and study of topological phenomena in quantum dynamics, including the exploration of topological phase transitions [116], the measurement of topological invariants [117], and the simulation of topological phases and edge states [119]. For example, Kitagawa et al. [182] observed topologically protected bound states in photonic quantum walks; Asbóth [183] explored the role of symmetries in one-dimensional quantum walks; and Panahiyan and Fritzsche [184,185] simulated multiphase configurations, phase transitions, and edge states with quantum walks using a step-dependent coin. Quantum walks can also be used to simulate the topological phases in nonunitary systems. Mittal et al. [176] investigated the persistence of topological phases in non-Hermitian quantum walks. They extended the one-dimensional split-step quantum walk model to a nonunitary quantum walk and demonstrated the persistence of topological phases. In addition, nonunitary Floquet operators have been used to explore the topological properties of non-Hermitian systems. By imposing PT symmetry, Xiao et al. [119] realized and investigated Floquet topological phases driven by PT-symmetric quantum walks. Xu et al. [186] explored the dynamic topology hidden in a periodically driven system using a quantum walk. They experimentally classified quenched quantum walks using the dynamic Chern number, which provides an intrinsic method for classifying quenched quantum walks. They also demonstrated the relationship between the dynamic Chern number and quasi-equilibrium topological bulk invariants associated with quenched quantum walks between different topological phases. In addition, they experimentally observed that split-step quantum walks can be characterized using a dynamic topological order parameter and measured this parameter in quantum walks [187].

Quantum walks are also used to simulate and understand complex biochemical processes such as photosynthetic energy transfer, the behavior of biological molecules such as proteins and DNA, and chemical reactions. Mohseni et al. [14] used a quantum walk to simulate the energy-transfer process in a photosynthetic system. Quantum walks can enhance the efficiency of energy transfer and conversion [188], which is crucial for energy harvesting and utilization in biological systems. Hoyer et al. [189] showed that there is a limit to the quantum speedup in these processes. Quantum walks can also be used to simulate the protein–DNA target search and DNA sequence assembly process [190,191], and it has been shown that they can improve the efficiency and accuracy of this search and assembly. Varsamis and Karafyllidis proposed a quantum-walk-assisted algorithm for peptide and protein folding prediction [191], which is important for understanding protein function and drug design. The essence of chemical reactions is the process of interactions between molecules, and quantum walks have been used to simulate these interactions to obtain a better understanding of the mechanisms and properties of chemical reactions. Chia et al. [192,193] explored the use of quantum walks in coherent chemical kinetics, developed reaction operators for radical pairs, and found that quantum walks can be used to model and predict the behavior of radical pairs in this system. Overall, the use of quantum walks for biochemical simulations can lead to new insights and possible breakthroughs in fields such as drug discovery and bioengineering.

Other quantum information tasks

Quantum walks have been extensively studied in the field of quantum information processing and have been used as toolboxes for the preparation, manipulation, characterization, and transmission of quantum states (quantum information). Various quantum-walk-based protocols for quantum communication and routing have been developed. A key advantage of using quantum walks in quantum information processing is their ability to encode and process quantum information in a highly controlled and tunable manner. Quantum walks have thus been explored in various tasks of quantum information processing (Fig. 8A to D), including entanglement generation [194–196], PST, quantum state measurement [197,198], quantum teleportation [199], quantum communication [200,201], and quantum cryptography [202].

Quantum entanglement is a key resource for quantum information processing. Quantum walks have been shown to be a powerful tool for generating and manipulating quantum entanglement. By controlling the evolution of quantum walks, the necessary entanglement can be generated. In 2013, Vieira et al. [195] proposed a dynamically disordered quantum walk designed to maximize the entanglement between 2 particles by introducing randomness into the evolution of the quantum walk. Their quantum walk can generate more entanglement than other types of quantum walks, and the entanglement it generates can be controlled by adjusting its parameters. Gratsea et al. [203] proposed a scheme for preparing hybrid maximally entangled states of 2 qubits by controlling the evolution of a quantum walk on a one-dimensional lattice, which involved encoding the target state into the initial state of the walk and controlling the walk evolution using a sequence of unitary operations. Using a DTQW, arbitrary superposition states for 2 qubits can be prepared [194]. Panda et al. [204–206] proposed various methods for applying DTQWs on graphs to generate entangled states. They designed a graph structure and quantum walk dynamics to maximize the entanglement between the quantum walker and internal DOFs. These methods have considerable potential for application in quantum information processing. In addition, quantum walks have been used to control the degree of entanglement between particles and generate entangled states with specific properties, such as maximal entanglement [195,196]. Furthermore, quantum walks can be used to study the properties of entangled states and to test the principles of quantum mechanics. For example, Rohde et al. [207] studied the entanglement dynamics of DTQWs and showed that the entanglement between the walker and environment can exhibit quasiperiodic behavior. Melnikov and Fedichkin studied the entanglement properties of the quantum walks of interacting fermions on a cyclic graph [18]. Quantum entanglement also arises between the coin and position in DTQWs [208–210], and recent experimental research shows that disorders can

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enhance the entangling ability of quantum walks [211]. This characteristic can be considered an indicator of the topological phases in quantum walks, according to [212].

The ability to determine the quantum state of a system accurately is crucial for many applications in quantum information processing. Quantum walks have great potential and advantages for the characterization and measurement of quantum states. First, quantum walks can be used to realize generalized and nonlocal quantum state measurements. In 2013, Kurzynski and Wojcik proposed that quantum walks can be viewed as generalized measurement devices [213] and demonstrated that a one-dimensional DTQW can be used to implement a generalized measurement in terms of a positive operator value measure (POVM) on a single qubit. Bian et al. [197] and Zhao et al. [198] used one-dimensional photonic quantum walks to realize POVM measurements of a single qubit. In addition, quantum walks can be used to achieve efficient quantum state reconstruction and tomography. Titchener et al. [214] used 2-photon Thomson scattering and quantum walks to implement the tomography of 2-photon states. They employed a hybrid quantum walk within on-chip coupled waveguide arrays as the measurement process and successfully reconstructed the input 2-photon density matrix. Hou et al. [215] achieved deterministic collective measurements using photonic quantum walks. They used a collective symmetric informationally complete POVM realized through a photonic quantum walk to perform qubit state tomography with unprecedented accuracy.

Quantum walks have also been explored as tools for quantum state transmission and for applications in quantum communication including quantum networks, quantum teleportation, and quantum key distribution. It is possible to transmit quantum states over long distances by encoding information regarding the state of the quantum walker. Targeting quantum communication applications, Yang et al. [200] and Chen et al. [201] proposed a novel DTQW approach for quantum network communication and presented a quantum multi-unicast communication scheme and a PST scheme over a butterfly network and an inverted crown network, respectively. Shang et al. [216] proposed quantum communication protocols based on quantum walks with 2 coins, where information is encoded in the coin state and transferred to any target position using 2 coin operators. Srikara and Chandrashekar [217] developed 2 quantum direct communication protocols, namely, a quantum secure direct communication protocol and a controlled quantum dialogue protocol, using DTQWs on a cycle graph. Panda et al. [218] proposed a new quantum direct communication protocol that utilizes the entanglement generated during the evolution of k-cycle DTQWs. In quantum teleportation applications, Wang et al. [219] proposed a generalized quantum teleportation protocol based on quantum walks with 2 coins, where an unknown qubit state can be teleported using quantum walks on a line and on a cycle with 4 vertices. This protocol can transmit any unknown d-dimensional state without the prior entangled state, making it more flexible than existing d-dimensional state teleportation protocols. In addition to single-qubit teleportation, quantum walks can also realize multiqubit teleportation. Li et al. [199] proposed a multi-particle quantum-walk-based teleportation scheme where the entanglement between walkers and their respective coins is generated by step operators in multi-particle quantum walks. This protocol allows for the flexible selection of the transmission path and enables more efficient transmission of quantum states. Moreover, quantum walks can also be used to implement a quantum key distribution protocol. Vlachou et al. [220] proposed a quantum key distribution scheme based on quantum walks that includes verification procedures against full man-in-the-middle attacks and provides provable unconditional security.

In the domain of quantum cryptography and security applications, quantum walks have been extensively explored for designing novel secure schemes and for attacking various cryptographic schemes. For example, quantum walks have been used in quantum image encryption [202,221–223], steganography [224–226], generating high-quality random numbers [227,228], quantum cryptanalysis [229], and attacking lattice-based cryptography [230]. Color images can be encrypted using controlled 1-particle quantum walks [202], 2-particle quantum walks [223], 2-dimensional quantum walks, and quantum coding. Quantum walks can also be used in combination with Gray code and Henon maps for cloud-based image encryption [231]. Quantum walks have also been applied in steganography [224–226] to achieve high security and can be used for cloud-based image steganography and e-healthcare platforms. Several studies [232–234] have proposed quantum-walk-based security protocols that can be used to protect data and information in various scenarios such as 5G networks and Internet of Things (IoT)-based smart cities. Quantum walks can also be used to attack cryptographic schemes. Kaplan et al. [229] proposed a quantum-walk-based differential and linear cryptanalysis method that can be used to break some traditional symmetric cryptography algorithms. Lattice-based cryptography is a leading candidate for postquantum cryptography. The shortest vector problem is crucial for the cryptanalysis of lattice-based cryptography. Chailloux and Loyer proposed a heuristic algorithm based on quantum walks to solve this problem, which considerably improved the running time of the algorithm [230]. Another common problem in cryptanalysis is collision finding, which has been extensively studied using both classical and quantum algorithms. To improve the efficiency of the algorithm in finding multiple collision pairs, Bonnetain et al. [235] introduced a chained quantum walk algorithm that considerably reduced the complexity of the algorithm.

Graph-theoretic applications

The underlying Hamiltonian that determines the evolution of quantum walks is directly associated with the structure of a graph, where, for example, in the CTQW each vertex of the graph encodes a quantum basis state, and each edge represents a possible transition between 2 quantum basis states. Quantum walks are thus a promising tool not only for graph-theoretic problems but also for various network applications, which they can map to related graph-theoretic problems (Fig. 8E to I). Quantum walks possess distinct characteristics on a graph compared with classical random walks and enable efficient graph structure explorations such as searching for marked vertices and ranking vertex importance. Quantum walks are particularly effective in identifying the structural differences between graphs and have been intensively studied for graph-comparison applications. Furthermore, various network applications have been studied by mapping onto graph-theoretic problems and addressed using quantum walks. Here, we summarize recent advancements in quantum walks used in graph-theoretic and network applications.

Compared to classical random walks, quantum walks are more efficient at exploring graph characteristics because they

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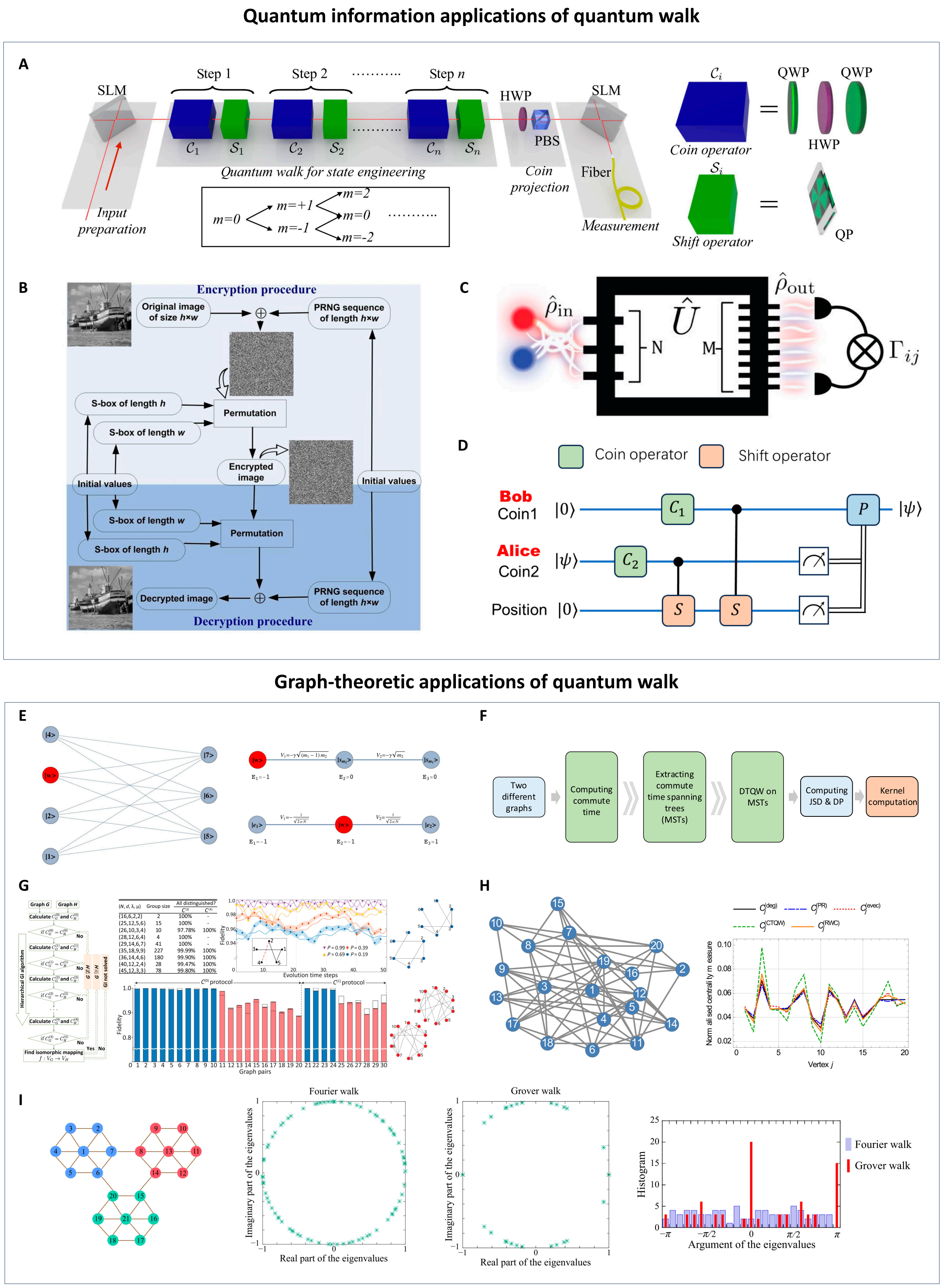

Fig. 8. Examples of quantum information processing and graph-theoretic applications of quantum walk. (A) Scheme for proposed implementation of quantum walk state-engineering protocol using the OAM and SAM of a photon. Reprinted with permission from [194]. Copyright 2017 by the American Physical Society. (B) General framework for quantum-inspired cascaded DTQW image encryption technique, reproduced from [227]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (C) Diagram of a hybrid quantum walk for 2-photon tomography, reproduced from [214]. (D) Quantum teleportation with 2-coin quantum walks on a line, based on [219]. (E) Quantum-walk-based spatial search on complete bipartite graph $K_{4,3}$ with solution node $|w\rangle$, reproduced from [241]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/. (F) The framework to compute the similarity between 2 complete weighted graphs using quantum-walk-based algorithm, based on [282]. (G) Experimental demonstration of quantum-walk-based GI algorithm. From [62]. Copyright the authors, some rights reserved; exclusive licensee AAAS. Distributed under a CC BY-NC 4.0 license http://creativecommons.org/licenses/by-nc/4.0/. Reprinted with permission from AAAS. (H) Vertex centrality measure of randomly generated Erdős-Rényi graph $G(20,0.3)$. Reprinted with permission from [256]. Copyright 2017 by the American Physical Society. (I) DTQW on complex networks for community detection on a prototypical 3-community network, reproduced from [274]. Distributed under a CC BY 4.0 license http://creativecommons.org/licenses/by/4.0/.

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perform quantum walk evolution on a graph. It has been shown that it is possible to achieve faster hitting and mixing times than with classical random walks [236–238]. This enables more accurate estimation of the spectrum and characterization of related properties such as connectivity and expansion properties. The spectrum of a graph generally indicates the essential features and properties of the graph, such as its diameter, degree distribution, and clustering coefficient [239]. Based on this, quantum-walk-based algorithms for searching for marked vertices, ranking vertex centrality, and other structural exploration tasks have outperformed their classical counterparts in different aspects. In 2003, Childs and Goldstone [7] first proposed a CTQW-based algorithm for spatial search problems (i.e., problems related to searching for marked vertices in graphs) and showed that quantum walks can achieve a quadratic speedup over classical algorithms for searching for a marked vertex on an unweighted graph of N vertices, where the complexity of the quantum walk algorithm is $O(\sqrt{N})$, but that of the classical algorithms is $O(N)$. It has been proven that a spatial search using a quantum walk algorithm is optimal for almost all graphs [240]. Several other studies have investigated CTQWs used in spatial search problems [24,25,241–244]. Janmark et al. [242] demonstrated that global symmetry is not necessary for fast quantum search using CTQWs. They proposed a new algorithm that achieves the same speedup as the standard Grover search algorithm using a nonsymmetric Hamiltonian. Wong [243] proposed a variant of Grover search using lackadaisical CTQWs that allows the quantum walker to rest occasionally during the search, thereby reducing resource requirements. Chakraborty et al. [245] discussed the optimality of spatial search via a CTQW and provided the necessary and sufficient conditions for optimal quantum search. Furthermore, quantum-walk-based algorithms have been used to search for marked vertices in weighted graphs [246–248] and dynamic graphs [249–251], and marked edges in graphs [252]. In addition to CTQW models, discrete quantum walk models, including the Szegedy walk, staggered quantum walk, and coin-based quantum walk, have also been shown to solve spatial search problems [26,34,35,253]. Quantum-walk-based search is attractive because it is expected to have useful properties (e.g., robustness to noise and ease of physical implementation) [251], and various experimental demonstrations have been presented. For example, using a bulk optics quantum system [124], Qu et al. experimentally demonstrated deterministic search on star graphs via quantum walks. Using a programmable silicon photonic chip, Qiang et al. [62] implemented a quantum-walk-based search on various graphs for both single and multiple marked vertices. They experimentally demonstrated, on a large-scale fully programmable quantum walk system, a quantum-walk-based search on graphs with 10 to 210 vertices [38].

In addition to searching for marked vertices, quantum walks show great potential for ranking vertex centrality. Vertex centrality is an integral tool in graph theory and network analysis and can be used to quantify the importance of each vertex. A higher vertex centrality measure indicates more importance. The vertex centrality measure has been widely used in ranking webpages on the Internet, for example, in the well-known PageRank algorithm, and in other applications such as identifying critical infrastructure nodes in social and urban networks. The PageRank algorithm was first proposed by Paparo et al. [254,255] based on SQW models. It is more sensitive than classical algorithms: it can highlight secondary hubs and resolve the degeneracy of low-lying nodes in the network [255]. An alternative quantum centrality measure using a CTQW model was also proposed [256]. It requires a smaller Hilbert space than Szegedy-quantum-walk-based algorithms. The CTQW-based vertex centrality ranking algorithm was extended to centrality measures for directed networks [257] and weighted graphs [258]. Experimental demonstrations of these algorithms include ranking vertices on directed graphs using bulk optics quantum systems [259,260] and testing quantum centrality ranking for scale-free networks of 55 vertices using a fully programmable silicon quantum photonic processor [38]. The experimental results achieved high fidelities with theoretical predictions.

Quantum walks have also demonstrated their effectiveness in identifying structural differences between graphs and are used for several types of graph-comparison problems, such as distinguishing nonisomorphic graph pairs, measuring similarity between graphs, and solving graph classification. The GI problem is the problem of determining whether 2 graphs have the same structure. It is thought to be neither an NP-complete nor a polynomial-time problem, and the best proven general algorithm is quasi-polynomial-time [261]. Several quantum-walk-based GI algorithms have been proposed, demonstrating the potential of quantum walk for solving GI problems [8–10,62,99,262–268]. These algorithms differ in terms of the type of quantum walk model that is used (i.e., discrete-time or continuous-time), number of particles involved, presence of particle interactions, localized inhomogeneities, and methods of constructing graph certificates. The single-particle CTQW model achieved an improved distinguishing ability for strongly regular graphs (SRGs) with 64 vertices by adding phases to the edges [62], while both interacting and noninteracting multi-particle CTQWs, especially for 2 bosons with interaction [9] and 4 fermions with noninteraction [99], can also distinguish nonisomorphic SRGs on the same scale. Strong distinguishability also appears in the single-particle discrete model. For example, as the level of the search-based signature increases, the isomorphism algorithm can obtain a stronger distinguishing ability, even for SRGs with up to 64 vertices [268]. It is noteworthy that although none of the proposed quantum-walk-based GI algorithms have been proven analytically to be able to distinguish all graphs in polynomial time, their capability of distinguishing nonisomorphic graphs has been tested by numerous numerical simulations on wide classes of graphs. Moreover, some of the algorithms, such as the CTQW-based GI algorithm, have been extensively experimentally demonstrated on fully programmable silicon photonic quantum walk processors [38,62], where the sizes of the experimentally tested graphs are up to 210 vertices [38]. Based on the distinguishability of nonisomorphic graphs, quantum walks can provide an effective measure of the similarity between graphs. There are 2 ways to use quantum walks to measure graph similarity: one is to use a similar method for calculating the fidelity between graph certificates that are directly constructed through the output probability distribution of the evolved states, and the other is to use the complete quantum state to compute graph kernels [269]. Quantum Jensen–Shannon divergence and related methods [270,271] show strong separation ability and have become popular methods for computing graph kernels and have been applied to both DTQW [269] and CTQW [272] models. Furthermore, computing the similarity matrix of a graph set as a key procedure can be directly used in classical classification

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models, leading to better performance in graph classification problems [269,271].

Based on studies on graph-theoretic quantum walk algorithms, quantum walk algorithms can be used in various fields for additional practical applications, such as network routing [239], social network analysis [273], community detection [274], and information propagation modeling [275]. In general, these applications can be modeled as graph-theoretic problems, and quantum walk algorithms can be used to find optimal solutions with speedup over classical algorithms or to explore complex dynamics and in-depth structural analysis via quantum walk dynamics. In the domain of network routing, a network can be modeled as a graph, where the vertices in the graph represent network routers or switches and edges represent the physical links connecting these devices. In a study by Zhan et al. [239], the scheme for realizing quantum routing was based on a controllable PST via DTQWs. In the field of social networks, by modeling users as vertices and social relationships between users as edges, complicated social networks can be mapped into large-scale graphs, and quantum walks can be applied to explore and analyze user behavior and social trends [273], which helps with in-depth analysis of the structure and dynamics of social networks. For example, quantum walks have been shown to define specific centrality metrics in terms of node occupation on single-layer and multilayer networks and to identify leaders in criminal networks [276]. In addition to information networks and social networks, quantum-walk-based algorithms have been proposed to solve problems in other networks, including traffic networks [277], unmanned aerial vehicle (UAV) communications [21], and sensor networks [278]. Specifically, a method for multiscale characteristic analysis for online car-hailing traffic volume with quantum walks was proposed, demonstrating the application of quantum walk algorithms in traffic optimization [277]. A coin-driven Hadamard quantum walk model [21] was proposed to identify the important edges of undirected complex networks and was deployed in a dynamic complex network involving a typical communication scenario found in UAV swarms to select important UAV nodes in a dynamic network.

Conclusion and Outlook

In this review, we have summarized the theories and characteristics of quantum walks, introduced the progress of physical implementations of quantum walks, and described quantum-walk-based algorithms and applications. Quantum walks represent a promising theoretical framework for application-specific quantum computing while holding the potential for universal quantum computing. The power of quantum walk computing systems over classical computers has been well demonstrated via the boson sampling task—as a particular multi-particle quantum walk sampling task. Moreover, with recent developments in the physical implementations of quantum walks, particularly in the integrated quantum photonics systems, important advances in both scale and programmability are demonstrated for quantum walk simulations and applications—most of which target problems of practical interest. This suggests that quantum walk models show a feasible path for building a practical and useful NISQ computer in the near future.

Despite this rapid progress, some challenges remain in the realization of practical quantum walk computing systems. One major obstacle is to devise quantum walk algorithms. This requires further investigation of various quantum walk models and in-depth research of their characteristics, for example, to understand their roles in achieving quantum computational advantages. Another challenge is to continuously scale up the physical implementations of quantum walks while improving programmability. For example, in integrated quantum photonics systems, the scale-up of quantum walks depends on both the number of evolving photons and the size of the Hamiltonian. Thus, increasing photon number becomes critical, and large-scale but low-loss reconfigurable optical networks are also core requirements, together with high-efficiency photon detection. Furthermore, although quantum walks may not be used for targeting fault-tolerant quantum computing at the current stage, methods for implementing quantum walks with error correction or fault tolerance are necessary, considering that the potential large-scale quantum walks for practical interests would require simulations with high precision. To this end, it may be necessary to investigate error mitigation or error correction techniques in implementing quantum walks and also to explore quantum walk algorithms under noisy conditions. Although these challenges require continuous efforts to solve, the field of quantum walk computing is vigorously developing, and it paves the way to a foreseen future for quantum computing.

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