Exploring complex graphs using three-dimensional quantum walks of correlated photons

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Graph representations are a powerful concept for solving complex problems across natural science, as patterns of connectivity can give rise to a multitude of emergent phenomena. Graph-based approaches have proven particularly fruitful in quantum communication and quantum search algorithms in highly branched quantum networks. Here, we introduce a previously unidentified paradigm for the direct experimental realization of excitation dynamics associated with three-dimensional networks by exploiting the hybrid action of spatial and polarization degrees of freedom of photon pairs in complex waveguide circuits with tailored birefringence. This testbed for the experimental exploration of multiparticle quantum walks on complex, highly connected graphs paves the way toward exploiting the applicative potential of fermionic dynamics in integrated quantum photonics.

INTRODUCTION

Complex networks occur across many different fields of science, ranging from biological signaling pathways and biochemical molecules exhibiting efficient energy transport (1) to neuromorphic circuits and social interactions in the ever-expanding World Wide Web (2). In general, such structures are modeled by graphs, whose complexity is dictated by the number of nodes and linkage patterns between them. Crucially, any physical representation of a graph is constrained by the fact that both of these need to be arranged in three-dimensional (3D) space. A marked example of the resulting scaling behavior, which is highly unfavorable for physical simulation, is the human brain, in which the already staggering number of 80 billion neurons is dwarfed by the 100 trillion synapses enabling the flow of signals between them (3). Despite the comparably miniscule number of nodes, discrete quantum systems face a similar challenge: Complex network topologies with a high degree of connectivity allow for potent applications (4) such as efficient multipartite quantum communication (5) or search algorithms (6, 7), but the physical implementation of such networks has—so far—been constrained to two dimensions.

The transport properties of connected graphs are usually studied in the framework of quantum walks (QWs). The paradigmatic case of a linear 1D chain has been implemented on a wide range of different networks ranging from biological systems (22–24) to graph theory problems (21, 25) and enables quantum search algorithms (26). Simultaneously leveraging both methods—multiple walkers and 2D single-particle graphs—brings the experimental realization of graphs with even higher complexity into reach (27). Unfortunately, spatial dimensions are a rather sparse commodity, a fact that is often exacerbated by practical limitations of technological platforms. Internal degrees of freedom of the walkers can mitigate these constraints by providing artificial dimensions (28). In the context of (classical wave) photonics, this strategy has enabled the implementation of specific scenarios via coupled sets of physical states (29, 30) or additional parameter dependencies in the system dynamics (31). The development of methods that are applicable to multiple walkers and genuinely increase the dimensionality of any physically implemented underlying graph remains an open challenge of crucial importance.

In this work, we demonstrate controlled QWs of correlated photons on 3D graphs. We realize the graph structure by means of a novel hybrid approach: 2D photonic lattices of spatially coupled waveguides are inscribed into fused silica by femtosecond laser writing (32), while one synthetic dimension is encoded in the photons' polarization. The dynamics within the synthetic dimension are established by harnessing the intrinsic birefringent properties of the elliptical waveguides that historically have been used as polarization active cores of individual single-mode optical fibers (33). By appropriately rotating the waveguides’ respective fast principal axes with respect to an external reference frame, continuous coupling between the two orthogonal polarization states takes place. In this vein, a single waveguide yields coherent population oscillations between the polarization modes (Fig. 1A). Whereas the external reference frame is arbitrary for an isolated core, the spatial arrangement of coupled waveguide removes this ambiguity. As such, lattices can be transformed into bilayer versions of themselves by an appropriate orientation of their elliptical cores (Fig. 1B). Notably, following this strategy to implement higher-dimensional graphs naturally gives rise to hypercube (HC) symmetries that have recently been predicted to leave their distinct signature on the evolution of correlated photon pairs (34). To discern the fingerprints of quantum interference, we use the nonclassicality $v = C_{\text{ind}}/C_{\text{dis}} - 1$, contrasting the measured coincidence count rates between indistinguishable ($C_{\text{ind}}$) and distinguishable

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photons ($C_{\text{MS}}$), respectively. We further examine conditions for the selective suppression ($\nu < 0$) or enhancement ($\nu > 0$) of output states, revealing bosonic and fermionic behavior on certain subgraphs, respectively. Last, we show that our technique allows for the control of both strength and sign of the coupling along the synthetic dimension and use negative couplings to selectively induce partial breaking of the graph’s HC symmetry. Our approach opens new avenues for the experimental exploration of quantum dynamics on highly complex graphs that play an essential role in numerous disciplines of science.

**RESULTS AND DISCUSSION**

To illustrate the working principle, we first show that the hallmark of two-particle interference, the Hong-Ou-Mandel (HOM) effect (35), arises in the polarization degree of freedom of a single waveguide. Direct laser-written waveguides in fused silica are intrinsically birefringent (36) and therefore can be individually described by the Hamiltonian

$$\hat{H} = \beta_s \hat{a}_s^\dagger \hat{a}_s + \beta_f \hat{a}_f^\dagger \hat{a}_f \tag{1}$$

with the bosonic annihilation (creation) operators $\hat{a}_s^{(1)}$ for photons on the slow/fast principal axis with propagation constant $\beta_{s/f}$, respectively. As schematically shown in Fig. 2A, these axes may be oriented at an angle $\alpha$ toward the horizontal/vertical (H/V) frame of reference (37). Any value of $\alpha$ that deviates from integer multiples of $\pi/2$ then entails dynamics in the polarization states of photons propagating along the $z$ direction according to the Heisenberg equation of motion (see section S1 for details)

$$i \frac{d}{dz} \begin{pmatrix} \hat{a}_H^\dagger \\ \hat{a}_V^\dagger \end{pmatrix} = \begin{pmatrix} \beta - \Delta \cdot \cos 2\alpha & \Delta \cdot \sin 2\alpha \\ \Delta \cdot \sin 2\alpha & \beta + \Delta \cdot \cos 2\alpha \end{pmatrix} \begin{pmatrix} \hat{a}_H^\dagger \\ \hat{a}_V^\dagger \end{pmatrix} \tag{2}$$

where $\beta = (\beta_s + \beta_f)/2$ describes the mean propagation constant and $\Delta = (\beta_s - \beta_f)/2$ represents the strength of birefringence. Notably, this mathematical structure is fully equivalent to the description of the dynamics in a coupled and detuned two-waveguide system. In our polarization-coupling regime, the counterpart of the propagation constants’ mismatch, $\Delta \cdot \cos 2\alpha$, and coupling strength, $\Delta \cdot \sin 2\alpha$, can both be adjusted via the birefringence $\Delta$ (36) and the rotation angle $\alpha$ (37). Here, the case of $\alpha = 45^\circ$—entailing equally large propagation constants for the H/V modes—appears particularly interesting because the system behaves analogously to a phase-matched directional coupler, or beam splitter, with a tunneling amplitude $t = \sin (z \cdot \Delta)$, depending on the propagation length $z$. Similar to conventional couplers (38), the performance of this component can be evaluated by measuring the quantum interference (35) between the polarization states. To this end, a polarization-duplexed input state $|H,V\rangle \equiv \hat{a}_H^\dagger \hat{a}_V^\dagger |0\rangle$ is synthesized from photon pairs generated by spontaneous parametric down-conversion (SPDC) and injected into a polarization-maintaining (PM) waveguide ($\alpha = 0$), in which a rotated section with angle $\alpha = (45.2 \pm 1.2)^\circ$ and length $L$ is embedded (see Fig. 2B). As the time delay $\tau$ between the photons at the injection facet is varied, the coincidence counts of two avalanche...
coupling strengths between the waveguides. Details on how birefringence establishes the additional dimension of the graph structure are provided in section S2. By choosing the waveguide spacing such that $\kappa = \Delta$, the resulting square lattice constitutes a 2D HC (34) for which the unitary transfer matrix after a coupling length $L = \pi/(4\Delta)$ reads

$$U = \left( \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \right)^{\otimes 2}$$

where $(\ldots)^{\otimes 2}$ denotes the tensor square applied to the transfer matrix of a two-site coupler with equal output amplitudes for a single-site excitation, also designated as HC symmetry factor. In our experiment, this is accomplished for a propagation length $L = 6.92$ cm. We investigate the collective dynamics of two-photon input states for all possible arrangements with, at most, one photon per site. After the transformation governed by the square lattice, the polarization components are separated by two on-chip polarization beam splitters (PBSs), with the photons subsequently detected by APDs. For distinguishable photons, the equally strong couplings between the

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**Fig. 3. Square lattices in a single spatial dimension.** (A) A pair of birefringent waveguides with slow axes at $\alpha = 45^\circ$ implements a square graph structure with coupling strengths $\kappa = (\kappa_f + \kappa_s)/2$ (averaged coupling strength between slow/fast axes) between waveguides 1 and 2, and $\Delta = |\beta_f - |\beta_s|/2$ between polarizations H and V. (B) Measured coincidence matrix of two distinguishable photons. For coupling parameters $\kappa = \Delta$, classical (single-particle) dynamics yields a nearly uniform distribution after a propagation length of $L = \pi/(4\Delta)$. (C) Coincidence rates for indistinguishable photons. In addition to the count rates (height), the nonclassicality is color-coded to indicate enhancement (red) and suppression (blue) by quantum (two-particle) interference. (D) Illustration of the self-inverse symmetry operations $\Sigma_i$, $\Sigma_2$, and $\Sigma_3$ on the 2D HC graph, leaving the two-photon arrangements (indicated by red spheres) invariant. (E) Nonclassicality for combinations of initial-final photon arrangements captured by the suppression laws associated with $\Sigma_1$, $\Sigma_2$, and $\Sigma_3$. The red (blue) squares indicate enhanced (reduced) probabilities of the corresponding input-output transition. (F) Clockwise ($\alpha = +45^\circ$) and counterclockwise ($\alpha = -45^\circ$) rotated principal axes implement a square lattice with negative coupling strength between two sites. For equal coupling strengths $\kappa = \Delta$ (c coupling strength between fast and slow axes of different waveguides) and propagation length $L = \pi/(4\Delta)$, we measure the coincidence rates for (G) distinguishable and (H) indistinguishable photon pairs.
lattice sites result in a uniform output probability distribution across the entire lattice (Fig. 3B). In contrast, as illustrated by the color-coded nonclassicality in Fig. 3C, for indistinguishable photons, destructive and constructive quantum interference causes full suppression (\( \nu \approx -1 \)) and pronounced enhancement (\( \nu > 0 \)), respectively. Upon closer examination, \( \nu \) appears closely related to the three self-inverse symmetries \( \Sigma_1 \) (mirror symmetry of the polarization coupler), \( \Sigma_2 \) (\( \pi \)-rotation of the square lattice), and \( \Sigma_3 \) (mirror symmetry of the waveguide coupler) of the HC graph illustrated in Fig. 3D: In accordance with the HC suppression law (39–41), the symmetry operation that leaves the input state invariant determines the suppression of four output states (different ones for each symmetry), while the detection probability of all other output states appears enhanced compared to distinguishable particles (cf. Fig. 3E).

The suppression of the \( \Sigma_1-S_1 \) and \( \Sigma_3-S_1 \) input-output combinations is closely related to HOM interference in the polarization or waveguide coupler, respectively. In this vein, photons are launched and observed in coupled sites and tend to bunch in one of the two sites irrespective of joint changes to the waveguide and polarization. The other cases arise from the interference of all photon-pair amplitudes traversing both lattice dimensions. As predicted by the HC suppression laws (see section S3), phase bookkeeping of all two-photon trajectories for the \( \Sigma_1-S_2 \), \( \Sigma_2-S_1 \), \( \Sigma_2-S_3 \), and \( \Sigma_3-S_2 \) input-output combinations reveals pairwise occurring paths with a phase difference of \( \pi \) and therefore, fully destructive quantum interference emerges (34).

In addition to increasing the dimensionality of lattices, Eq. 2 allows for even more general coupling scenarios: Combining waveguides with clockwise and counterclockwise rotated fast axes (see Fig. 3F), the polarization coupling terms acquire opposite signs, thereby providing a direct route to implement negative coupling strengths without the need for complex background lattice engineering or ancillary waveguides (42, 43). Notably, an \( \alpha = \pm 45^\circ \) arrangement also enables coupling between the \( V \)-polarized mode of one waveguide to the \( H \)-polarized mode of the other, and vice versa (see section S4 for details). Following this approach, we implement a polarization-encoded square lattice in which one of the polarization couplings has a negative sign, thereby breaking the underlying symmetry of the graph with special implications: Individual photons cannot be found on the diagonally opposite site of their starting position as a consequence of destructive interference caused by the different signs of coupling strengths. The resulting output statistics for distinguishable and indistinguishable photons are shown in Fig. 3 (G and H, respectively) and clearly differ from those obtained with positive couplings only. Because of the absence of photons on specific sites, for each input arrangement, the nonclassicality in Fig. 3H indicates suppression only for a single output state, whereas all other output states show no substantial fingerprints of quantum interference (\( \nu \approx 0 \)).

In a final set of experiments, we implement a 3D QW. An equilaterally coupled triangle of identical, birefringent waveguides (Fig. 4A) is transformed into a triangular prism whose unitary transfer matrix reads

\[
U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \otimes A
\]

(4)

where \( A \) is the transfer matrix of the triangular subgraph (see section S2 for details). Compared to Eq. 3, the tensor power of the HC symmetry factor is reduced by 1, and in general, only a single HC dimension is established in the polarization degree of freedom.

The input state \( |H_1, V_1\rangle \) (one \( H \)- and one \( V \)-polarized photon injected into waveguide 1) is invariant under the HC symmetry, as indicated by the mirror-symmetric projection into the polarization subspace in Fig. 4B. The polarization subspace contains a two-site coupler that plays the dominant part for the observed quantum interference (Fig. 4C): Output states with one photon in each \( H \) and \( V \) polarization (shown in the central layer of the 3D two-photon graph in Fig. 4C) appear suppressed, such that both photons must exit the structure in the same polarization state (top and bottom.
layers in Fig. 4C). In contrast, the input states $|H_1, H_2\rangle$ (see Fig. 4D) and $|H_1, V_2\rangle$ (see Fig. 4F) break the mirror symmetry in the polarization subspace and the HC symmetry–induced suppression of quantum states vanishes. For instance, $|H_1, H_2\rangle$ partially suppresses the probability of finding both photons in different waveguides and, at the same time, enhances bunching behavior of orthogonally polarized photons in the same waveguide (Fig. 4E). This property is inextricably linked to the bosonic QW on the triangular graph in the waveguide subspace in Fig. 4D. These observations are independent of the polarization, because single-photon hopping in the polarization subspace in this case only accumulates irrelevant phases for the two-photon interference and the influence of the HC structure vanishes (see section S3 for details). The same applies if the photons are launched in the input state $|H_1, V_2\rangle$ and subsequently observed both in the same polarization (H or V). In this case, only one photon changes the site in the polarization subspace and accumulates an irrelevant phase for quantum interference. Consequently, the top and bottom layers of the two-photon graph in Fig. 4G exhibit the same signatures of quantum interference as for the input state $|H_1, H_2\rangle$, which are only affected by the spatial two-photon dynamics. The input state $|H_1, V_2\rangle$ leads to a purely fermionic anti-bunching behavior for output photons with different polarizations (details are provided in section S3): Both photons, despite being bosons, inevitably end up in different waveguides, as evidenced by the full suppression and enhancement of the corner and remaining nodes in the central layer of the two-photon graph in Fig. 4F, respectively. For different output polarization, both photons either maintain or change their respective polarizations. Whereas maintaining the polarization does not introduce additional phases to the two-photon wave function, the joint polarization change can be interpreted as a permutation operation in the two-photon state in the waveguide subspace. The associated phase shift of $\pi$ gives rise to antisymmetric features of the two-particle wave function (44). In other words, the two bosonic walkers behave as fermionic walkers on the equilateral triangular waveguide lattice and adhere to the degeneracy prohibition expressed by the Pauli principle.

Notably, this division into bosonic and fermionic behavior is a direct consequence of the underlying HC structure and, as such, is not restricted to the triangular subgraph geometry investigated here: The same characteristics would hold for any other subgraph structure. Thus, the HC suppression law and the Pauli principle are the general mechanisms leading to the suppression of output states on the bilayer lattice (Fig. 5). In turn, specifically designed waveguide lattices (e.g., Fig. 3A) can selectively instantiate suppression mechanisms on the basis of bosonic or fermionic two-particle interference on the waveguide subspace.

The exploration of quantum dynamics on complex graphs plays an essential role in numerous disciplines of science. However, as the dimensionality increases, their experimental implementation becomes an ever more challenging task. We introduced a novel approach to expand the dimensionality of photonic lattices by using the polarization degree of freedom as an additional synthetic dimension that is applicable to current approaches for increasing the vertices’ connectivity in a spatial configuration (45, 46). As demonstrated by the observation of HOM interference in a single waveguide with appropriately tailored birefringence, the dynamical features introduced by the additional dimension are in perfect agreement with the characteristic

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**Fig. 5. Summary of forbidden and allowed output states.** Two photons are launched in different polarization sites (each photon position is indicated by a red node) and in different waveguides (right column) or in the same waveguide (middle column). We classify the possible final two-photon arrangements associated with their input state and their observed hallmarks of quantum interference in allowed (red frame) and forbidden states (blue frame) and same (middle row) and different (bottom row) output polarization states.

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**Fig. 6. Experimental setup.** (A) Correlated photon pairs are generated by type I SPDC. A BiBO crystal is pumped with a focused laser beam. The two horizontally polarized photons and the pump beam are separated with two prisms. After passing spectral filters, the photons are collected by PM fibers. The time delay $\tau$ between the photons is set by a delay stage. (B) The generated photon pairs are launched either on the fast or on the slow axes of the fibers in the PM fiber array. After the photons evolve in waveguide arrangements of two or three waveguides with rotated principal axes, they pass an integrated PBS on a second sample. In the end, the photons are collected with multimode (MM) fibers and detected with APDs.
quantum dynamics expected from spatial dimensions. In further proof-of-principle experiments, we observed quantum interference in fully controlled QWs of correlated photons on 3D graphs, a long-standing goal in quantum photonics. Beyond increasing the dimensionality of a given graph configuration, our technique naturally allows for the implementation of negative couplings without the need for any ancillary structures (42, 43). Along similar lines, polarization-coupled lattices can readily establish anti-bunching of photons—a key ingredient for probing complex fermionic QWs and harnessing their unique suppression behavior beyond conventional methods based on polarization-entangled two-photon sources that explicitly allocate fermionic or bosonic statistics according to an input state’s chosen exchange symmetry (47, 48). As a direct result from the here established framework, a number of fascinating opportunities arise beyond the context of correlated QWs: The quantum dynamics (both single-particle and multiparticle) of bilayer 2D materials can be emulated on wave packets evolving on complex graphs becomes experimentally accessible by using bright light pulses and the Kerr nonlinearity. Last, graphs with periodic boundaries or nontrivial topologies (49) as well as further topological questions such as the graph isomorphism problem can now be addressed more efficiently on optical platforms.

MATERIALS AND METHODS

Waveguide fabrication and classical characterization

We fabricate nearest-neighbor coupled waveguide circuits using the direct laser writing technique (32). Femtosecond pulses at \( \lambda = 800 \) nm with a 200 – kHz repetition rate were focused in fused silica with a 40× (NA = 0.65) or 20× (NA = 0.35) objective to fabricate the lattices for the HOM experiment (see Fig. 2) or the 2D and 3D QWs (see Figs. 3 and 4, respectively).

The rotation of the principal axis of a waveguide is realized by triplicated waveguides with a transverse offset of 3 and 5 \( \mu \)m oriented at an angle of 31° and 10° with respect to the horizontal plane for the 40× and 20× objective, respectively. We determine the orientation of the principal axis \( \alpha \) as well as the strength of birefringence \( \Delta \) with the method of two crossed polarizers (50). Simultaneously rotating the orientation of the first and second PBS by \( \theta \) (this maintains the crossed orientation of the polarizers), the intensity ratio of the transmitted light \( I_T \) and total intensity \( I_{\text{total}} \), measured with two photo diodes, reads

\[
\frac{I_T}{I_{\text{total}}} = \sin^2 (2(\theta - \alpha)) \sin^2 (L \cdot \Delta)
\]

with the length \( L \) of the waveguide. The angle \( \alpha \) can now be determined by the minimum in the recorded data. Using different lengths \( L \) of the 45° rotated part (e.g., realized to record the data in Fig. 2C) and fixed positions \( \theta = 0° \), the relatively transmitted intensity follows

\[
\frac{I_T}{I_{\text{total}}} = \sin^2 (L \cdot \Delta)
\]

so that \( \Delta \) can be reconstructed from the measurement.

Bi-photon creation and experiment

For the generation of photon pairs, we used a type I SPDC source (see Fig. 6A). A BiBO crystal is pumped by a 100 – mW laser diode (Coherent OBIS, continuous wave) at \( \lambda_p = 407.5 \) nm. This produces wavelength-degenerate horizontally polarized photon pairs at \( \lambda_s = 815 \) nm, which are collected by PM fibers and subsequently routed to the sample. We adjust the delay \( \tau \) in between the arrival times of the two photons at the sample with a delay stage. Indistinguishable photons are obtained by setting \( \tau = 0 \), whereas delays \( |\tau| > 1 \) ps yield distinguishable photons: According to the Gaussian fit of the HOM dips in Fig. 2C, a 1 – ps delay results in bunching of less than 0.7% photon pairs, which is negligible compared to the counting error in the case of less than 10,000 counts. For the characterization of the photons’ indistinguishability, we record the HOM dip that reaches a visibility of up to \( (92.3 \pm 1.1)\% \) as measured with a fiber-based beam splitter.

Our experimental setup (see Fig. 6B) allows us to launch photons from an SPDC source with either horizontal (H) or vertical (V) polarization. This feature is enabled by fiber mating sleeves that align the fast axis of the PM fiber from the SPDC source to either the fast or the slow axis of the PM fiber array with a pitch of 127 \( \mu \)m leading to the waveguide chip. Inside the sample, the laser-written waveguides start with a curved interface section to adiabatically reduce their transverse distance to the value associated with the desired spatial coupling. In this fan-in section, the principal axes are aligned to the PM fibers, such that they maintain H and V polarization. In contrast, the main section of the chip contains spatially coupled waveguides with rotated principal axes, which induce specific polarization coupling behavior and the desired lattice dynamics. Last, we implement one on-chip PBS (51) for each waveguide of our lattice. The functionality of this section is implemented by coupled pairs of waveguides with a precise mismatch of coupling strengths for H- and V-polarized light, respectively. In addition to the separation of polarizations, the individual PBSs are also gradually separated from each other. To avoid bending losses that might systematically skew the results of the photon counts, we choose a length of 7.10 cm for this fan-out. Each PBS was implemented to exceed a polarization contrast of 98% (classical characterization) in the respective output waveguides. The same PBS structure was designed to be used for all lattices investigated in this work.

SUPPLEMENTARY MATERIALS

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/7/9/eabc5266/DC1

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