Observation of topological phenomena in a programmable lattice of 1,800 qubits

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The work of Berezinskii, Kosterlitz and Thouless in the 1970s1,2 revealed exotic phases of matter governed by the topological properties of low-dimensional materials such as thin films of superfluids and superconductors. A hallmark of this phenomenon is the appearance and interaction of vortices and antivortices in an angular degree of freedom—typified by the classical XY model—owing to thermal fluctuations. In the two-dimensional Ising model this angular degree of freedom is absent in the classical case, but with the addition of a transverse field it can emerge from the interplay between frustration and quantum fluctuations. Consequently, a Kosterlitz–Thouless phase transition has been predicted in the quantum system—the two-dimensional transverse-field Ising model—by theory and simulation3–5. Here we demonstrate a large-scale quantum simulation of this phenomenon in a network of 1,800 in situ programmable superconducting niobium flux qubits whose pairwise couplings are arranged in a fully frustrated square-octagonal lattice. Essential to the critical behaviour, we observe the emergence of a complex order parameter with continuous rotational symmetry, and the onset of quasi-long-range order as the system approaches a critical temperature. We describe and use a simple approach to statistical estimation with an annealing-based quantum processor that performs Monte Carlo sampling in a chain of reverse quantum annealing protocols. Observations are consistent with classical simulations across a range of Hamiltonian parameters. We anticipate that our approach of using a quantum processor as a programmable magnetic lattice will find widespread use in the simulation and development of exotic materials.

Richard Feynman’s vision of simulating quantum systems with a quantum computer6,7 has motivated the field of quantum information since its inception. In the absence of large-scale programmable universal quantum computers, advances in quantum simulation are bound by available technology. Nevertheless, remarkable progress has been made using near-term approaches such as ultracold atoms8, superconducting qubits9, including superconducting and superfluid films22, trapped atomic gases10 and hybrid tin–graphene Josephson junction arrays23. KT phase transitions have, however, been observed in many systems including superconducting and superfluid films22, trapped atomic gases10 and hybrid tin–graphene Josephson junction arrays23. Here we exhibit this phenomenon in a large-scale programmable quantum simulation. We perform this simulation using a superconducting QA processor consisting of 2,048 radio-frequency superconducting quantum interference device (SQUID) flux qubits fabricated as an integrated circuit, in which the Hamiltonian terms \( h_i \) and \( J_{ij} \) are specified with programmable on-chip control circuitry16–18. The topology of the available non-zero coupling terms \( J_{ij} \) consists of a regular bipartite grid. On this programmable substrate we define a sequence of frustrated square-octagonal lattices having a cylindrical boundary condition (Fig. 1a), with the largest system using 1,800 qubits (see Methods). This lattice features chains of four ferromagnetically coupled qubits. In the large ferromagnetic (FM) coupling limit, the low-energy description of this lattice follows the same Landau–Ginzburg–Wilson theory as the widely studied4–5,24–26 triangular antiferromagnetic (AFM) lattice (Fig. 1b). We therefore use the same analytic machinery, which is valuable even outside the large FM coupling, low-temperature limit.

Central to this analysis is a mapping from each plaquette in the triangular lattice to a two-dimensional pseudospin that can be represented by a complex number \( \psi \). This gives the local angular degree of freedom in each plaquette, including vortices and antivortices, that can emerge. To first-order perturbation in the small–\( J / J_0 \) limit, an AFM triangle has six degenerate ground states, each consisting of an up-spin \( | \uparrow \rangle \) and a down-spin \( | \downarrow \rangle \). On this programmable substrate we define a sequence of frustrated square-octagonal lattices having a cylindrical boundary condition (Fig. 1a), with the largest system using 1,800 qubits (see Methods). This lattice features chains of four ferromagnetically coupled qubits. In the large ferromagnetic (FM) coupling limit, the low-energy description of this lattice follows the same Landau–Ginzburg–Wilson theory as the widely studied4–5,24–26 triangular antiferromagnetic (AFM) lattice (Fig. 1b). We therefore use the same analytic machinery, which is valuable even outside the large FM coupling, low-temperature limit.
corresponding set of six perturbative ground states that require four-qubit chains to be in delocalized superpositions of their computational basis states $|↑↑↑↓⟩$ and $|↓↓↓↑⟩$. Thus the addition of quantum fluctuations selects an ordered subset from the highly degenerate ground-state manifold, reducing entropy and imposing long-range correlations; this phenomenon is a form of ‘order by disorder’ $^4$, and naturally divides the spins into three sublattices categorized by their magnetization in the six perturbative ground states. The sublattice magnetizations $m_1$, $m_2$ and $m_3$, defined as the average of $⟨σ_z⟩$ over spins in the sublattice, give a complex order parameter $^5$

$$\psi = m e^{iθ} = (m_1 + m_2 e^{i2π/3} + m_3 e^{i4π/3})/\sqrt{3}.$$  

In the absence of open boundary effects, $\psi$ is simply the average of pseudospin $ψ$ over all plaquettes in the system. Figure 1d, e shows pseudospins in the triangular lattice; a full explanation is given in the Methods.

In the square-octagonal lattice, we use the same order parameter with the three sublattices defined according to the natural mapping: two FM-coupled spins must be in the same sublattice, and two...
AFM-coupled spins must be in different sublattices. Figure 2a shows plots evaluated on each plaquette for an output state from the QA processor. Figure 2b shows the phase diagram of the square-octagonal lattice in the $T$–$J$ plane, which resembles that of the triangular lattice (see Methods). At high temperature the system is in a disordered paramagnetic phase. As $T$ drops, for $T < 1.76$, the system enters a KT phase, in which vortices and antivortices form bound pairs. At even lower temperature, the system transitions into an ordered phase, where $U(1)$ symmetry is broken and $\psi$ concentrates around the six low-temperature clock states (white circles in Fig. 1c, see Methods). While the generation of vortices and antivortices relies on competing quantum and classical fluctuations in the TFIM, the upper KT phase transition occurs in the error bars. We estimate statistics using both an ordered initial state and a random initial state ($\psi = 0.20$ and $\psi = 0.26$) values of $\psi$. Brightness indicates relative frequency of values; $\psi$ shows rotational $U(1)$ symmetry consistent with the expected paramagnetic and KT phases (see Methods).

We experimentally probe values of $s$ between 0.20 and 0.30 at physical temperature $T$ between 8.4 mK and 21.4 mK. Figure 3b shows the expectation (m) as a function of $s$ for the 1,800-spin lattice (lattice width $L = 15$) at 8.4 mK, compared with estimates from continuous-time path-integral quantum Monte Carlo (QMC) simulations as detailed in the Methods. In agreement with QMC, QA shows a peak in (m) close to where the QA schedule cuts through the KT phase in the large system limit, with a small shift caused by the open boundary condition and finite-size effects—the phase diagram is determined using toroidal rather than cylindrical instances (see Methods). For $s > 0.24$, QA shows good agreement with QMC. For smaller $s$, the dynamics of the system is fast (see Methods) and the system orders during the 1-µs quench, leading to an overestimate of (m); results are almost unchanged between $s = 0$ and $s = 0.2$.

The histogram of the complex order parameter $\psi$ is plotted in Fig. 3c for two points along the QA schedule. As $s$ increases from 0.20 to 0.26, both QA and QMC show the emergence of order; $\psi$ concentrates around a ring with the characteristic $U(1)$ symmetry of the two-dimensional XY model despite the discrete $\mathbb{Z}_2$ symmetry of the Ising model\cite{24,25,27}.

In the thermodynamic limit, the KT phase transition is marked by a change of correlation decay from exponential to power-law at the critical temperature. In the critical phase, correlations $C_{ij}$ decrease with distance $x_{ij}$ as $C_{ij} \propto x_{ij}^{-\eta}$ with an exponent $b$ bounded above by the universal two-dimensional XY critical exponent $\eta = 1/4$. At finite sizes, the transition is expected to be broadened, and the apparent transition point can be affected by boundary conditions. To probe the onset of critical behaviour we study correlations in the complex field $\psi$ on the plaquettes of the largest lattice on 1,800 spins; correlation is measured
as $C_{ij} = \langle \text{Re}(\psi_i^* \psi_j^\dagger) \rangle$ on plaquettes along the periodic dimension, halfway between the open boundaries.

Figure 4a shows $C_{ij}$ as a function of distance for two temperatures at $s = 0.26$, with good agreement between QMC and QA. The absolute shift between QMC and QA correlations is explained by evolution during the quench (see Methods). As temperature decreases, correlations decrease, approaching power-law decay: the quality of power-law fit on distances 1 to 5—where boundary effects are minimal—improves as temperature decreases. This is shown in Fig. 4b for $s = 0.25$ and 0.26, near the peak of $(m)$ in $s$ (Fig. 3b). The exponent $b$ of this power-law regression decreases with temperature (Fig. 4c), reaching a minimum value of $b \approx 0.35$ for QA and $b \approx 0.32$ for QMC.

In the vicinity of the critical region, the same onset of power-law behaviour is expected for $(m)$ as a function of size with a halved exponent that is, $(m) \propto L^{-s/2}$. This is shown in Fig. 4d, where QA shows agreement with QMC over a range of system sizes. Scaling exponents of $b \approx 0.34$ and $b \approx 0.29$ for QA and QMC, respectively, are close to the values extracted from phase correlations in Fig. 4c.

We have presented a large-scale quantum simulation of an exotic phase of matter. Our experimental results show clear signatures of topological phenomena: a complex order parameter with rotational symmetry that respond as expected to changes in $T$ and $\Gamma$, and the onset of power-law scaling of correlations. Taken together, these constitute the experimental observation of topological order in a frustrated two-dimensional transverse-field Ising model, as theoretically predicted and simulated in QMC. Agreement with QMC over a range of system sizes and Hamiltonian parameters—independently extracted with no fitting parameters—validates the flux qubit implementation of the transverse-field Ising model at large scales.

The reverse annealing technique used in this work promises to greatly expand the utility of quantum annealing processors. The ability of a QA processor to reverse anneal from an input state allows us to validate convergence of our statistical estimators to a steady state, but its importance is far more general: quantum evolution of an input state is crucial to the implementation of hybrid quantum-classical algorithms. Quantum evolution Monte Carlo is perhaps the simplest such algorithm.

This programmable magnetic material has allowed us to study the many-body dynamics of matter that is time-consuming to simulate classically and difficult to implement physically. The methods used here can be applied to explore other exotic phases of matter in a variety of lattices. Several future developments will improve our simulation approach. First, greater qubit connectivity will allow more flexibility in lattice geometry and realization of fully periodic boundary conditions. Second, faster projective readout will enable more accurate sampling from systems with fast dynamics, and any advances in noise and control error will improve the accuracy of these simulations. And finally, with the addition of non-stoquastic couplings, quantum annealing processors could foreseeably simulate systems of which classical simulations are intractable even at modest scale.

**Online content**

Any Methods, including any statements of data availability and Nature Research reporting summaries, along with any additional references and Source Data files, are available in the online version of the paper at https://doi.org/10.1038/s41586-018-0410-x.

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METHODS

Pseudospin phase and topological features in the TFIM. In the TFIM, the triangular AFM lattice and fully frustrated square-octagonal lattice admit an approximate mapping to the two-dimensional XY model that is essential to the topological phenomena we observe. Here we provide a description of this mapping, which has its origins in the study of the stacked magnet\(^2\) and has since been described in the quantum case\(^3\).

We begin with a description of the XY model and the upper KT phase transition intersected by the QA schedule.

The two-dimensional XY model describes an interaction of classical spins. Each spin is a unit vector described by an angle \(\theta\). The interaction between spins is given by the XY Hamiltonian

\[
H = -J_{XY} \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)
\]

where the sum is taken over all coupled pairs of spins. The ground state of this system is one in which all spins are aligned (see Extended Data Fig. 1); note that the system described by equation (1) has continuous O(2) or U(1) symmetry.

In a ground state, the angle \(\theta\) does not change as we traverse a closed path in the plane in a clockwise direction. Given a perturbation of a ground state, \(\theta\) may fluctuate along this path but will not wind in a full rotation. A clockwise or anticlockwise winding is known as a vortex or an antivortex, respectively; these topological defects imply an excitation that diverges with the radius \(R\) of the encircling path:

\[
E_{\text{vortex}} = \pi J_{XY} \log \frac{R}{r}
\]

where \(r\) is the lattice spacing. The entropy \(S_{\text{vortex}}\) also grows proportionally to \(\log(R/r)\) since there are \((R/r)^2\) possible locations of the vortex in an area of \(R^2\). A competition of these two terms leads to a sign-variable expression for the free energy contribution of a vortex:

\[
\Delta F = E_{\text{vortex}} - TS_{\text{vortex}} = (\pi J_{XY} - 2k_B T) \log \frac{R}{r}
\]

The critical vortex unbinding temperature \(T_2\) at which the KT phase transition occurs is given by the sign change of \(\Delta F\):

\[
T_2 = \frac{\pi}{2k_B} J_{XY}
\]

Above this temperature, the free energy favours isolated vortices; below this temperature vortices and antivortices are attracted to one another and appear in bound pairs.

The mapping from the TFIM to the XY model arises from the interaction of frustration and quantum fluctuations. We first consider the effect of a perturbative transverse field on a single AFM triangle. In the classical case, the AFM triangle has six ground states. In each, one of two floppy spins can be flipped without changing the energy. Extended Data Fig. 2 shows two such states differing by a flip of spin 1. The addition of a perturbative transverse field \(\Gamma\) lifts this degeneracy, allowing a superposition of these two states in which spin 1 aligns with the transverse field. We denote this superposition by \(|\downarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle) / \sqrt{2}\) and note that this lowers the energy from \(0 - j - \Gamma\) to \(-\Gamma\).

To first-order perturbation, this quantum ground state is six-fold degenerate, with the three spins taking values \(|\uparrow\rangle, |\downarrow\rangle, |\pm\rangle\) in any permutation. We map these six states to the complex plaquette pseudospins \(\psi_i\) as described by equation (2):

\[
\psi_i = (\sigma_i^x + \sigma_i^y)^{2\theta_i} + (\sigma_i^x - \sigma_i^y)^{2\theta_i}
\]

This is shown in Extended Data Fig. 3 for the state \(-|\pm\rangle\). Pseudospins for six quantum and six classical states are shown in Extended Data Fig. 3d. Also shown are the classical excited states \(|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle\), which have \(\psi = 0\). As vanishing points of the pseudospin phase, these magnetized triangles correspond to vortices and antivortices in the lattice.

As shown in Fig. 1d, the triangular AFM lattice can be tiled with a single clock state, resulting in a pseudospin that is constant across the lattice. This tiling naturally divides the sites of the lattice into three sublattices, which we use to determine the complex order parameter \(\psi\) as in equation (3). The introduction of a twist in the pseudospin phase, as shown in Fig. 1e, leads to a state where both of the triangles contain no spin aligned with the transverse field. This excitation can be described in terms of an effective XY model on the dual lattice, with effective XY coupling proportional to \(\Gamma\). This is consistent with the linear scaling of \(T_2\) in \(s^2\) seen in the small-\(J\) limit\(^4\). The corresponding phase boundary in the square-octagonal lattice, which is defined by the energy splitting of four-qubit chains, has a quartic form as presented with the details of the phase diagram below. To compute the pseudospin of a plaquette in the square-octagonal phase we use all 12 spins in the three FM-coupled chains intersecting the plaquette, whether it is a square or an octagon.

The pseudospin emerges from the six perturbative ground states of an AFM triangle, and thus the XY pseudospin at low temperatures is related not to the U(1)-symmetric XY model, but to the six-state clock model with \(Z_6\) symmetry.

In the six-state clock model studied by Jose et al.\(^2\), there are three phases: as temperature drops from the paramagnetic phase, we first see the vortex unbinding KT transition described above. Then, at even lower temperature, the system enters an ordered phase where the complex order parameter concentrates around one of the six clock states. Throughout the critical phase between the paramagnetic and ordered phases, \(U(1)\) symmetry is observed because the symmetry-breaking term does not become relevant until the lower transition\(^6\). The same three phases are seen in the triangular\(^3\) and square-octagonal lattices in the TFIM (we map out the phase diagram later in the Methods section). Thus at the regions of the \((T_l, T_t)\) plane probed by QA experiments, the observation of \(U(1)\) symmetry is consistent with both QMC simulations and theory.

The effective pseudospin XY model is derived from the perturbative limit \(T \approx 0\), \(\Gamma \rightarrow 0\), and only serves to provide the universal properties in the large-system limit. While so it is an effective means of understanding the KT transition in the triangular and square-octagonal lattices, it cannot provide the non-universal details of the TFIM outside the perturbative regime, and even at intermediate system sizes its universal properties deviate noticeably from expected values\(^5\).

Quantum processor and experimental methods. The quantum annealing processor used in this work is a D-Wave 2000Q system operated in a non-annealing mode. Operating temperatures ranging between 8.4 ± 0.2 mK and 21.4 ± 0.2 mK are measured with a cryostat thermometer and independently verified using single-qubit susceptibility measurements.

We focus on the region of the annealing schedule between \(s = 0.20\) and \(s = 0.30\) (Extended Data Fig. 4a). In quantum annealing, the annealing parameter \(s\) is typically increased smoothly from 0 to 1, bringing the system from a single-well superposition to \(s = 0\) to a low-temperature classical system at \(s = 1\) (Extended Data Fig. 4b). In our experiments we take a different approach, using the reverse-annealing protocol described in section III.D of Lanting et al.\(^2\). In this protocol we initialize the system at \(s = 1\) with a classical state loaded into the qubits. We then reduce \(s\) quickly, bringing the system to the quantum model we want to simulate.

We let this model relax for a fixed evolution time, 65 ms except in the relaxation timing experiments (see Methods section ‘Non-equilibrium dynamics of QA and QMC’), before quickly quenching to \(s = 1\) (Extended Data Fig. 4c). The evolution time of 65 ms was chosen to be roughly as long as possible within the constraints of the control electronics, to ensure that the operating temperature is as low as possible.

Each call to the processor consists of 50 reverse anneals for all data in the main text, and between 50 and 200 reverse anneals in the relaxation timing experiments. In the relaxation timing experiments the same initial state is used for every reverse anneal. In all other runs, a single initial state (clock or random) is loaded for the first anneal, and each subsequent anneal is initialized with the final state of the previous anneal. This allows us to perform quantum evolution Monte Carlo to estimate the equilibrium statistics of the target system. From each processor call, we discard the first 25 of 50 samples as described in the main text. Data shown in the main text represent 480 processor calls (with the exception of Fig. 3c, which represents 720 processor calls) divided equally between clock initial state and random initial state, each of which is further divided equally between two physical embeddings of the lattice.

In the Monte Carlo runs, a single initial state (clock or random) is loaded for the first anneal, and each subsequent anneal is initialized with the final state of the previous anneal (Extended Data Fig. 4c). This allows us to perform quantum evolution Monte Carlo to estimate equilibrium statistics of the target system. From each processor call, we discard the first 25 of 50 samples as described in the main text. Data for additional temperatures and values of \(s\) are shown in Extended Data Fig. 5.

Compensation of qubit nonidealities. When \(\Gamma\) is small, the radio-frequency SQUID flux qubits faithfully model two-level Ising spins. Since our experiments are performed in a region of the schedule where \(\Gamma\) is large, behaviour deviates from a two-level Ising system. To mitigate this nonideality we make two adjustments.

The first adjustment is a compensation of transverse and coupling energy scales, which are given to high accuracy using eight energy levels per SQUID instead of the two levels of an ideal Ising spin\(^7\). Since order in the square-octagonal lattice arises via tunnelling of 4-qubit FM chains, our approach is to determine a compensation \(f(s)\) such that a chain of four FM-coupled 8-level SQUIDS at \(s\) has the same first eigengap \(E_1 - E_0\) as a chain of four FM-coupled 2-level SQUIDS at \(f(s)\). These gaps are shown in Extended Data Fig. 4d, and the compensation is shown in Extended Data Fig. 4e. To confirm that this shift in \(s\) makes sense as a compensation approach, we probe the spectra more generally by adding a bias on the first SQUID of the chain and examining the first three eigengaps in Extended Data Fig. 4f. The compensation approach is validated by the agreement of the first eigengap across a range of biases and \(s\) values. Higher energy levels, which show nonideality, are less important.

The second adjustment is a compensation of effective next-nearest-neighbour couplings. Beyond the issue of energy scales just addressed, the radio-frequency SQUID flux qubits in the QA processor provide an imperfect implementation of
Ising spins early in the anneal. The primary deviation is that every qubit mediates a coupling between any two of its neighbouring qubits. This introduces next-nearest-neighbour couplings, meaning that for any spins $i, j, k$, there is an effective coupling term $\chi_{ijk} J_{ijk}$ added to $H_{QA}$; the strength is denoted $\chi_{ijk}$ representing a normalized background susceptibility: $\chi_{ijk} = \mathcal{M}_{ijk} \chi_{ijk}$, where $\mathcal{M}_{ijk}$ is the maximum available AFM mutual inductance and $\chi_{ijk}$ is the physical qubit susceptibility. The value of $\chi_{ijk}$ varies from $-0.07 \pm 0.02$ early in the anneal to $-0.03 \pm 0.01$ late in the anneal where single-spin dynamics become apparent, as measured by independent experiments.

In the QA experiments, we compensate for $\chi_{ijk}$ based on the fact that FM couplers are most often unfrustrated in the systems studied. We consider the application of next-nearest-neighbour terms as a function applied to the coupling Hamiltonian $H_{QA}$ supplied to the processor, and seek a choice of $\chi_{ijk}$ such that $f(\chi_{ijk})$ approximates $\nu$ for some constant $\alpha > 0$. This gives us the following constraints on the classical Hamiltonians:

1. Any two chains have the same total coupling between them in $f(\chi_{ijk})$ and $\nu$.

2. If a chain has a single break (domain wall), the total strength of frustrated couplers is the same in $f(\chi_{ijk})$ and $\nu$. In the absence of boundary conditions, this coupling is $-1.8\mu$.

We use an iterative method to determine $\chi_{ijk}$ given an average AFM coupling strength $\rho$. It follows that $\alpha$ is a function of $\rho$ and $\nu$ (in turn, $\nu$ is a function of $\rho$). For $\rho = 0.95$ the value of $\alpha$ ranges monotonically from 1.27 at $s = 0.20$ to 1.13 at $s = 0.50$.

Embedding the square-octagonal lattice. The cylindrical topology of the square-octagonal lattice is realized as two square sheets coupled together at the top and bottom (Extended Data Fig. 6). In the processor used, the graph of available couplings is a $16 \times 16$ grid of eight-qubit complete bipartite ‘Chimera’ unit cells35; only a $7 \times 7$ block of cells is shown in Extended Data Fig. 6b. Each FM-coupled chain of four qubits consists of two unit cells and one qubit in each of two other unit cells. If the size of the unit cell was doubled, it would be possible to embed a toroidal square-octagonal lattice with fully periodic boundary conditions. The halving of the antiferromagnetic couplers on the open boundaries of the cylinder ensures that the classical ground-state space is highly degenerate and includes the ordered clock states (Extended Data Fig. 8a) as well as striped states (Extended Data Fig. 8b) in each orientation.

Calibration refinement. The QA processor was calibrated as a general-purpose quantum annealer, with the goal of good performance across a variety of inputs. Given our focus on one particular input type, we can improve performance by exploiting structure and symmetries in the input. After compensating for background susceptibility as described above, we exploit symmetries in the lattice.

The first symmetry is spin-flip invariance: since there is no longitudinal field, the expected magnetization of each spin in the absence of systematic biases should be zero. To maintain this degeneracy we apply flux-offset biases to qubits in a gradient descent method, greatly improving the distribution of qubit magnetic moments.

The second symmetry is rotational symmetry about the periodic dimension. For lattice width $L$ (with $4L^2$ 2L spins), each coupler is in an equivalence class of $2L$ rotationally equivalent couplers that should be frustrated equiprobably. More generally, two couplers should have the same statistics if there is a graph automorphism over the lattice that maps one to the other. We make fine adjustments to individual coupling terms to tighten the frustration distributions of these equivalence classes (Extended Data Fig. 7b).

There are no further trivial symmetries in the square-octagonal lattice; both the triangular lattice with semi-open boundary and the square-octagonal lattice with fully periodic boundary have richer automorphism groups that might be exploited in future research. The symmetries that we use for calibration refinement apply at every point in the phase diagram, so the calibration refinement used here does not result in overfitting.

Spin-bath polarization. The persistent current flowing in the qubit bodies during the QA protocol produces a magnetic field that can partially align or polarize the spin environment. For long evolution times, the polarized environment can produce sample-to-sample correlations, biasing the QA towards previously achieved spin configurations. To reduce sample-to-sample correlations, biasing the QA towards previously achieved spin environment. For long evolution times, the polarized environment can produce sample-to-sample correlations, biasing the QA towards previously achieved spin configurations.

To reduce sample-to-sample correlations, we introduce a pause (Extended Data Fig. 7b) which is then checked for consistency with the same experiment given a random initial state. Convergence of the Binder cumulant and moments of the order parameter are tested with respect to initialization in several different types of classical ground state. Error is determined self-consistently between independent runs; error bars on QMC results are 95% bootstrap confidence intervals. Pseudospin correlations are computed from 5120 classical states projected from QMC in ten independent runs. Experimental lengths are up to $2^{20}$ Monte Carlo sweeps.

Non-equilibrium dynamics of QA and QMC. We now turn our attention to the non-equilibrium dynamics of the system in relation to its QMC counterpart: continuous-time path-integral Monte Carlo with imaginary-time cluster updates described above. We measure evolution timescales by initializing each system in two classical ground states. The first is a clock state (Extended Data Fig. 8a) in which the scalar field $\psi_0$ is uniform and $m = 0$; the second is a striped state (Extended Data Fig. 8b) in which $\psi_0$ is staggered and $m = 0$. As evolution time of QA and QMC is increased, the expectation of $m$ at the end of a single evolution converges in expectation towards a single value regardless of initial condition (Extended Data Fig. 8c).

We compare the evolution time required by QA and QMC to sweep the clock-initialization and striped-initialization estimates of $m$ to within 0.3 of each other (Extended Data Fig. 8d). Both QA and QMC become slower as $m$ increases, as quantum and thermal fluctuations are reduced. The scaling of evolution time in $s$ is far steeper for QMC than for QA, indicating that in this case QMC provides accurate equilibrium statistics of the quantum statistics, but does not simulate the dynamics. To reduce these onerous QMC timescales we employed parallel tempering and developed a lattice-specific cluster update method (not used in Extended Data Fig. 8) — a future study will analyse the impact of these and other advanced methods.

Phase diagram of square-octagonal lattice. Here we provide evidence for the claimed phase diagram of the square-octagonal lattice. We show critical behavioural and give estimates of the upper and lower critical temperatures bounding the critical KT region in the phase diagram of the square-octagonal lattice, and give an estimate of the quantum critical point at $T = 0$. We follow the methods used by Isakov and Moessner36 on the triangular lattice. We study $L \times L$ lattices (on $4L^2$ spins) with fully periodic (toroidal) boundary conditions with $L$ ranging from 3 to 21. Our results are presented in Extended Data Fig. 9.

For a range of transverse fields we use two methods to determine the lower ($T_L$) and upper ($T_U$) critical temperatures using properties of the two-dimensional XY universality class.

First, we use the expected power-law decay of correlations—and consequently $m$—as system size increases. Within the critical region and for fixed $T$, $m$ is expected to scale as $L^{-\nu}$, with critical exponents $\eta = 1/9$ and $\nu_2 = 1/4$. From this we determine $T_L$ and $T_U$ using a power-law fit on values of $L$ between 6 and 21 (Extended Data Fig. 9).

Second, we additionally determine $T_1$ and $T_2$ by fitting our data to universal scaling curves. For the lower transition, we have

$$m L^\nu = m_0 (L^{-1} e^{-\chi L T})$$

where $m_0$ is a universal function, $\nu$ is a non-universal constant, and $T = (T_L - T_1)/T_1$ is the residual temperature approaching $T_1$ from below. For the lower transition, we have

$$\chi L T_1 \nu = \chi_{\nu} (L^{-1} e^{-\chi L T})$$

where $\chi_{\nu}$ is a universal function, $\nu$ is a non-universal constant, and $T = (T - T_2)/T_2$ is the residual temperature approaching $T_2$ from above. We expect universality in that these fits, $b \approx (1/9)/2$ and $c \approx 7/4$. 

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For the upper transition, we obtain good collapses for $\Gamma$ between 0.7 and 1.3. These values are in fairly good agreement with values of $T_1$ determined from $\eta$, as in the triangular lattice. For the lower transition, fitting is generally poor and we obtain only a reasonably convincing collapse for $\Gamma \in [1.1, 1.2]$ by discarding data for $L < 15$. Values of $T_1$ deviate noticeably from those given by $\eta$. A study of larger instances would clarify the picture.

Again extending from the triangular lattice, we anticipate a quantum phase transition consistent with the three-dimensional XY universality class with dynamical exponent $z = 1$ and universal exponent $\nu = 2/3$. To estimate the quantum critical point, we measure the normalized Binder cumulant

$$U = 2 \left(1 - \frac{(m^4)}{2\langle m^2 \rangle^2}\right)$$

We do so for system sizes up to $L = 15$ using inverse temperature $\beta(L, \Gamma) = 3.5 L^z/\Gamma$. The Binder cumulant $U$ crosses near a critical point $\Gamma_c \approx 1.76$. Scaling of $U$ in the vicinity of the quantum critical point collapses as $U L^{1/\nu} = (\Gamma - \Gamma_c)/\Gamma_c$ using $\nu = 2/3$. The dynamical exponent $z = 1$ was verified by fitting the peak susceptibility as a function of $L$.

The mapping between the square-octagonal model and the six-state XY model in the perturbative limit $\Gamma \to 0$ admits an effective XY coupling proportional to the tunnelling energy of a four-qubit FM chain; this will have a fourth-order polynomial form in $\Gamma$ (Extended Data Fig. 9f).

**Effect of quench.** The QA simulation generally shows good agreement with QMC in estimates of $\langle m \rangle$, consistent with the formation and annihilation of vortex–antivortex pairs. However, these excitations appear far less often in QA output states than in projected QMC states. Here we show that this can be explained by evolution during the 1-μs QA quench. As quantum and thermal fluctuations are reduced, tightly bound vortex-antivortex pairs are annihilated. Extended Data Fig. 10 compares the mean residual classical energy per spin of QA and QMC. QMC projected states have many more excitations than QA states. We model a local classical quench in QMC output by repairing classical excitations at the single-qubit level and four-qubit chain level. After this classical quench is applied to QMC output, residual energies of QMC states resemble those of QA states. Effect on $\psi$ is minimal. This is consistent with the hypothesis that similar annihilation of defects occurs during the QA quench. We therefore expect that faster QA quench should lead to a greater population of classical excitations—vortices and antivortices—in QA output.

**Statistical methods.** All error bars show 95% bootstrap confidence intervals over 1,000 bootstrap samples. For QA results in Figs. 3b and 4, independent confidence intervals are generated for the Monte Carlo estimators with ordered initial state and random initial state, and the union of these intervals is shown. For every data point analysed in Fig. 3c we also show the equivalent data points under reversal of all spins and/or rotation (but not flipping) of the cylinder. Thus we show 27,000 effective samples for QA and 30,720 effective samples for QMC.

**Data availability.** The datasets generated and analysed during this study are available from the corresponding author on reasonable request.

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Extended Data Fig. 1 | Topological features in the two-dimensional XY model. a, The ground state, in which all rotors have equal angle $\theta$, has continuous U(1) symmetry, as a universal rotation of $\theta$ will not change the energy of the system. b, c, A vortex or antivortex (b and c, respectively) is a point around which the angle winds (rotates completely) clockwise or anticlockwise, respectively, when traversing a closed loop around the point in a clockwise direction. Both the energy and the entropy of an isolated vortex or antivortex region of radius $R$ are proportional to $\log(R/r)$, where $r$ is the lattice spacing.
Extended Data Fig. 2 | Floppy spin aligns with the transverse field.

a, b. Two of six degenerate classical ground states differ by a flip of spin 1. c. With the addition of a perturbative transverse field $\Gamma$, spin 1 aligns with the transverse field in a symmetric superposition $|\rightarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$, reducing the energy from $-J$ to $-J - \Gamma$. Red and blue represent spin-up and spin-down, respectively.
Extended Data Fig. 3 | Pseudospins from classical and quantum states.

**a**, Each pseudospin $\psi_j$ is determined as a linear combination of basis vectors with weights given by $\sigma^z$ operators. **b, c**, the pseudospin of the clock state $|\uparrow\downarrow\rangle$ is $e^{i\pi/2}$. **d**, The six-fold-degenerate perturbative quantum ground states (white, with magnitude 1) and six-fold-degenerate classical ground states (black, with magnitude $2/\sqrt{3}$) admit twelve ‘clock’ pseudospins in the complex plane. Also shown are the classical excited states $|\uparrow\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\downarrow\rangle$, which have pseudospin 0 and therefore correspond to a vortex or antivortex.
Extended Data Fig. 4 | Annealing schedule and protocols. a, Unitless energy scales for transverse field $\Gamma$ and Ising couplings $J$ as a function of annealing parameter $s$, compared with temperature $T = 8.4$ mK (the inset is a detail of the region studied: $0.2 \leq s \leq 0.3$). b, Standard 16-$\mu$s forward anneal protocol given as $s(t)$, which increases linearly from 0 to 1. c, 16-$\mu$s evolution in a reverse annealing protocol, where $s$ drops from 1 to $s = 0.3$ over 3.5 $\mu$s, dwells at $s$ for 16 $\mu$s, and quenches to 1 over 1 $\mu$s. Experiments, with the exception of relaxation time measurements, are performed with 216 $\mu$s (65 ms) dwells at target model $s$. d, The first eigengap $E_1 - E_0$ for a chain of four FM-coupled SQUIDs given by a physically realistic 8-level SQUID model deviates from the gap given by the desired 2-level SQUID model of Ising spins. e, To compensate for this deviation, we determine a nonlinear shift in $s$ so that the gap of the chain of 8-level SQUIDS at $s$ matches the gap of the chain of 2-level SQUIDs at $f(s)$. This shift in $s$ is roughly 0.03 to 0.05 in the region of interest, and is reflected in the effective schedule (a). f, To evaluate this compensation more generally, we place a flux bias on the first device of the chain and compare the eigenspectra of the 8-level SQUID model at $s$ with the compensated 2-level SQUID model at $f(s)$, for three values of $s$. Agreement in the first eigengap is good across a range of biases and $s$ values.
Extended Data Fig. 5 | Convergence of quantum evolution Monte Carlo.

Our quantum evolution Monte Carlo sampling approach involves making a chain of 50 reverse annealing evolutions starting from an ordered state and a random state. At 8.4 mK, cooling of around 0.1 mK is observed during the first 25 evolutions. This cooling lowers $m$ at $s = 0.26$, as the lower temperature slows evolution during the 1-μs quench. The same cooling increases the order parameter at $s = 0.26$, where the lower temperature results in evolution of a more ordered model. Shown are experimental results for increasing values of $s$ (top row) and for $s = 0.26$ at increasing temperatures (bottom row). At $s = 0.30$, $T = 8.4$ mK, evolution is slow and the estimates of $\langle m \rangle$ are far from the equilibrium value of $\langle m \rangle$ after a single 65-ms evolution. Spin-bath polarization, which biases the estimators towards the initial condition at low temperatures, disappears as temperature is increased.
Extended Data Fig. 6 | Embedding a cylindrical lattice into the qubit connectivity graph. a, b, The cylindrical square-octagonal lattice with length $L = 6$ (a) is embedded into a region of the Chimera qubit connectivity graph (b). The embedding consists of two square sheets that are coupled together at the top and bottom. The largest instance studied with $L = 15$ uses 1,800 of the 2,048 qubits in the processor, with unused qubits along the outside boundary of the processor. FM couplers are in blue and AFM couplers are in red.
Symmetries in the lattice dictate that each qubit should have an average magnetization of zero (a) and that each AFM coupler should be frustrated with the same probability as other couplers in its rotational symmetry equivalence class of \(2L\) couplers (b). We use a gradient-descent shim method (code available from the corresponding author on reasonable request) to maintain degeneracy among qubits and equivalent couplers with flux offsets and small adjustments to specified coupling energies. Data are taken for \(L = 15\), with 1,800 qubits and 1,290 AFM couplers, over 120 experiments with and without shim. Both magnetization and correlation distributions are tightened substantially. Outliers in shimmed spin–spin correlation are symmetry classes near the boundary of the lattice.
Extended Data Fig. 8 | Evolution time required to converge from two distant initial states in an 1,800-spin lattice. a–c, We initialize the quantum simulation (QA) and the classical Monte Carlo simulation (QMC) with single-spin updates (that is, no cluster updates) in two classical ground states, shown for $L = 6$ with pink and blue representing up and down Ising spins, respectively. One is a clock state (a) with order parameter $m = 2/\sqrt{3}$. The other is a striped state (b), which has $m = 0$ and is far from other classical ground states in Hamming distance. As these initial states are evolved in either QA or QMC for increasing evolution times, $m$ converges towards a steady state (c) regardless of initial condition. The uptick of $m$ for long QA evolution may be a signature of on-chip cooling during evolution. d, The time required to converge $m$ for the two initial conditions to within 0.3 of each other increases with $s$, as thermal and quantum fluctuations drop and dynamics slow. This indicates that QMC simulates only the equilibrium statistics of quantum evolution—not the dynamics.
Extended Data Fig. 9 | Phase diagram of the square-octagonal lattice from Monte Carlo simulations with toroidal boundary conditions. a, b, We estimate the upper (a) and lower (b) KT phase transition via universal collapse of susceptibility data, varying temperature for several values of $\Gamma/J$ (shown: $\Gamma/J = 1.2$); lower collapse is imperfect. c, Power-law scaling of $m$ with $L$ at upper and lower critical temperatures with critical exponents from two-dimensional XY universality. Lines show power-law regression. d, Crossing of the normalized Binder cumulant for models with $\beta = 3.5L/J$ gives an estimate of the quantum critical point $\Gamma/J \approx 1.76$ (the inset shows the collapse of Binder cumulant across system sizes). e, From this data we derive a picture of the phase diagram of the square-octagonal lattice with $J_{FM} = -1.8J_{AFM}$. f, In the perturbative limit, the critical temperature of the square-octagonal lattice is determined by the energy splitting of four-qubit FM chains. Therefore, the perturbative phase boundary corresponding to the triangular lattice’s linear perturbative phase boundary has a quartic form (boundary shown is proportional to $\Gamma^4$, fitted by eye).
Extended Data Fig. 10 | Effect of classical quench on QMC samples.

a, Distributions of classical energy differ greatly between QA and QMC output, with QA giving much lower classical energies. b, When a local quench is performed on QMC output, removing local excitations at the single-qubit level and the four-qubit chain level, the energy distribution matches QA closely. c, Quenching increases $\langle |\psi| \rangle$ by 0.02 in these QMC samples. Samples are collected for $s = 0.26, T = 8.4 \text{ mK}$. 