

Digital quantum simulations of scattering in quantum field theories using W states

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High-energy particle collisions can convert energy into matter through the inelastic production of new particles. Quantum computers offer a route to simulating these out-of-equilibrium processes, but accessing post-collision dynamics and determining the abundance of produced particles remain challenging. Here we report evidence for inelastic particle production in one-dimensional Ising field theory using a digital quantum processor. We collide two wavepackets, each containing the lightest particle in the theory, and use the skewness of the measured energy density to identify an inelastic component containing one outgoing light particle and one heavier particle. The experiment uses 104 qubits and up to 5,589 two-qubit gates to access the post-collision dynamics. The computation relies on a quantum algorithm that extends protocols for efficiently creating W states—multipartite entangled states with a single excitation distributed across many qubits—to prepare the initial wavepackets. With mid-circuit measurements followed by operations conditioned on their outcomes, the circuit depth is independent of the wavepacket's spatial volume, rather than scaling polynomially as in previous methods. We construct wavepacket-preparation circuits for one-dimensional Ising and scalar field theories, the Schwinger model and two-dimensional Ising field theory.

Quantum computers promise to be powerful tools able to simulate the dynamics of strongly coupled quantum many-body systems^{1–4}. In many instances, these simulations are beyond the capabilities of even the most powerful supercomputers⁵. Quantum simulations of quantum field theories (QFTs) would enable first-principles studies of the behaviour of matter present in extreme astrophysical environments, high-energy particle collisions and the early universe^{6–12}. This pinnacle of *ab initio* scientific investigation, along with advances in quantum technologies, has motivated the first simulations of QFTs on quantum devices^{13–45}. Notably, quantum simulations of QFTs have been among the first to surpass the capabilities of exact statevector simulations^{46–54} and are strong candidates for a quantum advantage.

A fundamental process in QFTs is scattering, in which particles travel towards each other, collide and eventually form an asymptotic

state. The evolution of the quantum state throughout the collision encodes information about the interactions, particle content and mechanisms that govern dynamics in the theory. At the ultrarelativistic energies accessed in particle collider experiments, kinetic energy is converted into matter through the production of many particles. Predicting the abundances of particles produced in these processes, as well as their collective dynamics, is a forefront theoretical problem. In this work, evidence for particle production is observed for the first time in a quantum simulation of inelastic scattering. A key element of this simulation is a new algorithm for preparing the initial state, that is, single-particle wavepackets. The algorithm has two steps:

- (1) Prepare a state $|W(k_0)\rangle$ that establishes the spatial profile, momentum content and quantum numbers of the target wavepacket but has contributions from multi-particle states.

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- (2) Project $|W(k_0)\rangle$ onto single-particle eigenstates by minimizing the energy with symmetry-preserving quantum circuits. The energy minimum corresponds to the target wavepacket.

The initial state $|W(k_0)\rangle$ is similar to the W state⁵⁵ that has been well studied in quantum information science due to its robust entanglement structure and applications to quantum communication, sensing and optimization^{56–63}. Recent work has shown that W states can be prepared in constant circuit depth using mid-circuit measurement and feedforward (MCM-FF)^{64–67}. Inspired by techniques from refs. 68,69, we improve the W state preparation protocol in ref. 64 by removing the need for ancillas. We present an ancilla-free protocol for preparing W states in constant depth, and a straightforward generalization of this method is used to efficiently initialize $|W(k_0)\rangle$ in the first step of the wavepacket preparation algorithm.

The symmetry-preserving circuits that minimize the energy in step 2 are found using the variational algorithm ADAPT-VQE⁷⁰ running on classical computers. In the future, energy-minimizing circuits could be determined using ADAPT-VQE or a different algorithm with provable performance guarantees on a fault-tolerant quantum computer. Our wavepacket preparation algorithm can be applied to a wide range of lattice models. Furthermore, the required circuit depth is independent of wavepacket size and only scales with the correlation length. This is a substantial improvement over previous methods, which either incur an exponentially scaling classical computing overhead^{47,48} or require a circuit depth that scales polynomially with the wavepacket size^{14,32,71–74}.

We demonstrate the utility of this algorithm by constructing wavepacket preparation circuits in one-dimensional Ising field theory, scalar field theory, the Schwinger model and in two-dimensional Ising field theory. In one-dimensional Ising field theory, the circuits that prepare wavepackets on lattices with 100+ qubits are determined using a matrix product state (MPS) simulator. These wavepacket preparation circuits are then used to initialize a scattering simulation on 104 qubits of IBM's quantum computer *ibm_marrakesh*. For current hardware capabilities, we find that linear-depth unitary circuits are more practical for preparing $|W(k_0)\rangle$ than the MCM-FF method. The application of up to 45 steps of Trotterized time evolution (5,589 two-qubit gates) evolves the system well beyond the collision. The paths of the particles throughout the scattering process are identified from measurements of the energy density. The creation of a slow-moving heavy particle during the collision causes the energy density in the post-collision state to be skewed. The skewness is extracted from our quantum simulations and is evidence for inelastic particle production.

'Overview of the wavepacket preparation algorithm', 'Quantum simulations of scattering in one-dimensional Ising field theory' and the 'Discussion' constitute the main text of this Article and are designed to be read sequentially. 'Overview of the wavepacket preparation algorithm' provides a high-level overview of the wavepacket preparation algorithm. 'Quantum simulations of scattering in one-dimensional Ising field theory' presents results from using *ibm_marrakesh* to simulate inelastic scattering in one-dimensional Ising field theory. The 'Discussion' concludes and discusses prospects for a near-term quantum advantage in simulations of scattering. The Methods support the results presented in the Article. In particular, the constant-depth circuit that prepares $|W(k_0)\rangle$ is given in the 'A constant-depth circuit for initializing $|W(k_0)\rangle$ ' section of the Methods. Circuits that prepare wavepackets in one-dimensional Ising field theory are determined using an exact statevector simulator in the 'Quantum circuits for preparing wavepackets in one-dimensional Ising field theory' section in the Methods. In the 'Quantum circuits for simulating scattering in one-dimensional Ising field theory' section in the Methods, circuits that prepare wavepackets on large lattices in one-dimensional Ising field theory are constructed using a MPS circuit simulator. In the 'MPS simulations of scattering in one-dimensional Ising field theory' section in the Methods, they are used to simulate scattering with MPS. Details about the

experiments performed on *ibm_marrakesh*, including the error mitigation techniques used, are given in the 'Details on the simulations performed using IBM's quantum computers' section in the Methods. The 'Calculating skewness' section in the Methods shows how inelastic effects can be detected from the asymmetry in the outgoing energy density and explains our method for quantifying this with skewness. The Supplementary Information provides additional information and expands on discussions in the Methods.

Overview of the wavepacket preparation algorithm

A quantum simulation of particle scattering begins with the preparation of single-particle wavepackets. Our method prepares wavepackets of the lightest particles with given quantum numbers by minimizing the energy starting from a suitable initial state. The circuits that minimize the energy could be determined from running variational algorithms on a quantum computer. For one-dimensional systems these variational algorithms can instead be implemented using a MPS circuit simulator. Importantly, the energy minimization circuits can be made hardware-efficient by adapting the ansatz to the connectivity and native gate set of the target quantum computer. Therefore, this method is particularly advantageous for simulations on near-term quantum computers that are limited by circuit depth. For simplicity, this section focuses on preparing wavepackets in one-dimensional lattice QFTs.

Consider a system with a unique ground state that is invariant under time reversal and spatial translations, and has periodic boundary conditions (PBCs). Its Hamiltonian $\hat{H}$ is block diagonal, with each block labelled by a momentum k . If the Hamiltonian has a mass gap, the ground state and first excited state of the $k = 0$ block correspond to the vacuum and the lightest particle at rest, respectively. The lowest-energy states of the other $k \neq 0$ blocks are the lightest single-particle eigenstates with momentum k which we define as $|\psi_k\rangle$. The block-diagonal structure of the Hamiltonian is illustrated in Fig. 1, left. These properties of the Hamiltonian motivate a variational quantum algorithm for preparing single-particle wavepackets.

A wavepacket is a superposition of single-particle eigenstates that is localized around a position x_0 and a momentum k_0 . A wavepacket with a small spread in momentum space σ will have a large spread in position space $\sim \sigma^{-1}$ and will propagate for a long time as a localized particle. The wavepacket wavefunction is

$$|\psi_{\text{wp}}\rangle = \mathcal{N} \sum_k e^{-ikx_0} e^{-(k-k_0)^2/(4\sigma^2)} |\psi_k\rangle, \quad (1)$$

where $\mathcal{N}$ is a normalization factor. A consistent phase convention is necessary when defining the single-particle eigenstates $|\psi_k\rangle$ (Supplementary Section H). The sum runs over $k \in 2\pi n/L$, where L is the number of lattice sites, and n is an integer such that $k \in (-\pi, \pi]$. For systems with a dispersion relation that is monotonic in $|k|$, a wavepacket that propagates to the right (left) will have the bulk of its amplitude in eigenstates with $k > 0$ ($k < 0$). As a warm up, first consider the task of preparing $|\psi_k\rangle$.

The state $|\psi_k\rangle$ with $k \neq 0$ can be prepared in two steps. First, some state $|k\rangle$ that is in a definite momentum block of the Hamiltonian (that is, an eigenstate under spatial translations, $e^{-ikn}|k\rangle = e^{-ikn}|k\rangle$) is initialized. One simple choice for $|k\rangle$ is the superposition of all states related by translation to $|00 \dots 001\rangle$ weighted by the appropriate phase. This assumes a basis where $|00 \dots 001\rangle$ has the quantum numbers of the target single-particle state. For example, in scalar field theory, single-particle states are odd under the Z_2 symmetry that takes $\phi \rightarrow -\phi$. If one lattice site maps to one qubit, this state would be

$$|k\rangle = \frac{1}{\sqrt{L}} \sum_{n=0}^{L-1} e^{ikn} |2^n\rangle, \quad (2)$$

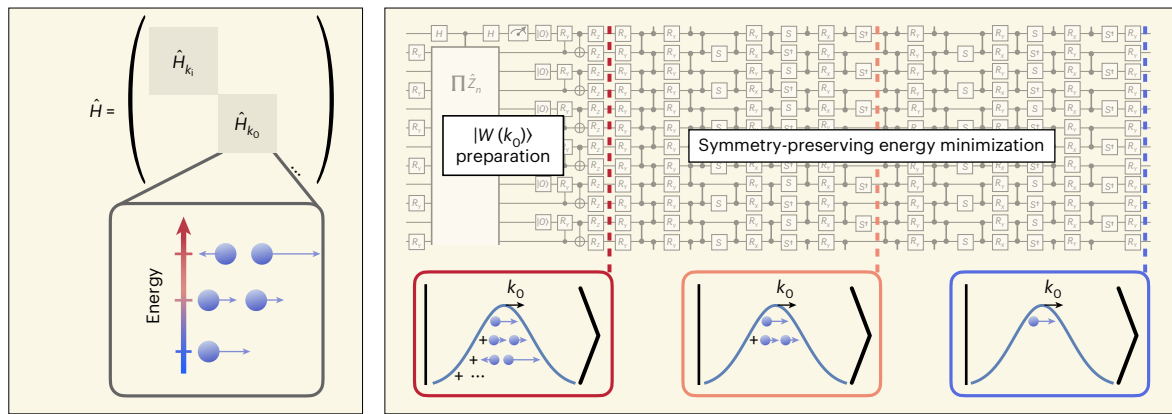


Fig. 1 | Wavepacket preparation using W states and symmetry-preserving energy minimization. Left: due to translational invariance, the Hamiltonian decomposes into blocks $\hat{H}_k$, each with definite momentum k . The lowest-energy state in each block corresponds to the single-particle momentum eigenstate $|\psi_k\rangle$. Higher-energy states can be interpreted as multiple particles with total momentum k (or heavier single-particle states not shown). Right: quantum circuits that prepare the target wavepacket $|\psi_{wp}\rangle$. First, the state $|W(k_0)\rangle$ is

prepared with a constant-depth circuit using MCM-FF (step 1). This initial state has the momentum content of the target wavepacket but incorrectly contains higher-energy components. Next, the energy is minimized using circuits that are translationally invariant, real and conserve other system-specific symmetries (step 2). These constraints preserve the momentum content of $|W(k_0)\rangle$ while projecting the wavefunction onto the desired single-particle states. The energy minimum corresponds to $|\psi_{wp}\rangle$.

where the state is specified by its binary value on L bits, for example, $|2^1\rangle = |00 \dots 010\rangle$. This state is in the correct k block of the Hamiltonian and has the long-range entanglement inherent to momentum eigenstates⁷⁵ but needs to be rotated to the lowest-energy state. A circuit that approximately implements this rotation $|\psi_k\rangle \approx \hat{U}(\theta_\star)|k\rangle$ can be determined by minimizing the energy

$$\hat{U}(\theta_\star) = \operatorname{argmin} \langle \psi_{\text{ansatz}} | \hat{U}(\theta)^\dagger \hat{H} \hat{U}(\theta) | \psi_{\text{ansatz}} \rangle, \quad (3)$$

where $|\psi_{\text{ansatz}}\rangle = |k\rangle$ and $\hat{U}(\theta)$ is a translationally invariant unitary operator $e^{i\hat{k}n} \hat{U}(\theta) e^{-i\hat{k}n} = \hat{U}(\theta)$ that depends on variational parameters θ . This circuit must also preserve the other quantum numbers of $|\psi_k\rangle$, and translational invariance ensures that the resulting state remains in the correct k block of the Hamiltonian. This forms the basis for a variational algorithm, and circuits that prepare $|k\rangle$ and minimize the energy can readily be constructed.

The generalization of this strategy to prepare $|\psi_{wp}\rangle$ begins with the initialization of some state $|W(k_0)\rangle$, which has the correct amplitude and phase in each k block of the Hamiltonian. A simple choice is a wavepacket built from $|k\rangle$,

$$\begin{aligned} |W(k_0)\rangle &= \mathcal{N} \sum_k e^{-ikx_0} e^{-(k_0-k)^2/(4\sigma^2)} |k\rangle \\ &= \sum_n e^{i\phi_n} c_n |2^n\rangle, \end{aligned} \quad (4)$$

where the magnitude of c_n follows a Gaussian centred at $n = x_0$. The special case of a uniform superposition is the W state⁵⁵. Using techniques from refs. 68,69 we improve the W state preparation circuits in ref. 64 and generalize them to prepare $|W(k_0)\rangle$. The circuit is given in the ‘A constant-depth circuit for initializing $|W(k_0)\rangle$ ’ section in the Methods and utilizes MCM-FF to prepare $|W(k_0)\rangle$ in two-qubit gate depth 7. The depth is independent of lattice geometry, system size and target wavepacket size. The use of W states for preparing wavepackets in analogue quantum simulations was recently proposed in ref. 76.

A simplified description of the circuit is the following: first, single-qubit rotations produce the state $|000 \dots\rangle + \sqrt{\delta}|W(k_0)\rangle + \delta|X\rangle$, where $|X\rangle$ contains states with two or more 1s in their binary representations, and δ is an input parameter. Next, the parity $\prod \hat{Z}_n$ (and only the parity) is measured using the constant-depth circuit from ref. 64. Post-selecting on odd parity prepares $|W(k_0)\rangle$ with infidelity $\mathcal{I} = \mathcal{O}(\delta^2)$ and succeeds with probability $p_{\text{success}} \geq 0.43\delta$ (assuming

$\delta \leq 1$). For large wavepackets, the success probability and infidelity are independent of wavepacket size (‘A constant-depth circuit for initializing $|W(k_0)\rangle$ ’ section in the Methods). The state $|W(k_0)\rangle$ has the momentum content of the target wavepacket but incorrectly contains components with two or more particles, as well as heavier single-particle components. This is illustrated by the first step in Fig. 1, right.

After preparing $|W(k_0)\rangle$, the wavefunction in each k block is rotated to the lowest-energy state while preserving its amplitude ($e^{-(k_0-k)^2/(4\sigma^2)}$) and phase (e^{-ikx_0}). The circuit that approximately performs this rotation $|\psi_{wp}\rangle \approx \hat{U}(\theta_\star)|W(k_0)\rangle$ is again determined from minimizing the energy in equation (3). Now, $|\psi_{\text{ansatz}}\rangle = |W(k_0)\rangle$, and $\hat{U}(\theta)$ is translationally invariant, real and conserves the other quantum numbers of $|W(k_0)\rangle$. Translational invariance preserves the amplitude of the initial state in each k block and reality preserves the phase. At a practical level, $\hat{U}(\theta)$ can be constructed from translationally invariant and imaginary operators $\hat{O}_j$ as $\hat{U}(\theta) = \prod_j e^{i\theta_j \hat{O}_j}$. Each of the terms $e^{i\theta_j \hat{O}_j}$ is then converted to a quantum circuit via Trotterization. Operators $\hat{O}_j$ generated from the Lie algebra of the Hamiltonian are particularly effective at minimizing the energy and guide the circuit design in this work. The energy minimization effectively projects out all unwanted multi-particle and heavy single-particle components of the $|W(k_0)\rangle$ wavefunction, leaving only the target single-particle wavepacket $|\psi_{wp}\rangle$. This is illustrated by the second step in Fig. 1, right.

This wavepacket preparation method can be applied to a wide range of lattice models in any finite spatial dimension. The required circuit depth is independent of wavepacket volume, provided that the qubit connectivity matches that of the target lattice. Supplementary Section B discusses the limitations and possible extensions of the wavepacket preparation method. In the next section, this algorithm is used to initialize simulations of scattering in one-dimensional Ising field theory on IBM’s quantum computers. In Supplementary Section B, it is applied to the preparation of wavepackets in one-dimensional scalar field theory, the Schwinger model and two-dimensional Ising field theory.

Quantum simulations of scattering in one-dimensional Ising field theory

The physics of the Ising model illustrates the complexity of quantum phenomena that can emerge from simple interactions. This has made it a target for quantum simulations, with recent demonstrations of

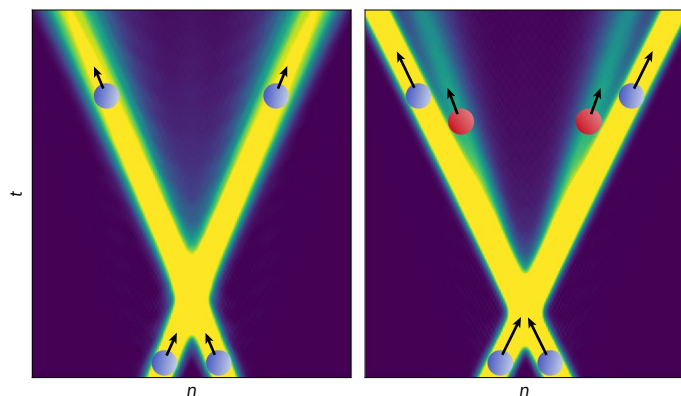


Fig. 2 | Low-energy versus high-energy collisions. A heat map of the energy density throughout the scattering process as a function of lattice position n and time t . Propagating particles are identified as beams of energy with a constant velocity. Left: the elastic scattering of two light $|1\rangle$ particles (blue), $11 \rightarrow 11$. Right: the inelastic process $11 \rightarrow 12$ that produces a heavy $|2\rangle$ particle (red).

many-body localization⁷⁷, discrete time crystals⁷⁸, Majorana edge modes⁷⁹ and string breaking³⁴. Our work focuses on the field theory that emerges when the Ising model Hamiltonian

$$\begin{aligned}\hat{H} &= -\sum_{n=0}^{L-1} \left[\frac{1}{2} (\hat{Z}_{n-1}\hat{Z}_n + \hat{Z}_n\hat{Z}_{n+1}) + g_x \hat{X}_n + g_z \hat{Z}_n \right] \\ &\equiv \sum_{n=0}^{L-1} \hat{H}_n,\end{aligned}\quad (5)$$

is tuned to criticality: $g_x \rightarrow 1$, $g_z \rightarrow 0$ and $L \rightarrow \infty$. The energy density $\hat{H}_n$ will be an important observable and is defined in the second line. The physics at the critical point is described by the conformal field theory (CFT) of a free, massless Majorana fermion. A family of Ising QFTs is reached by tuning to criticality, but keeping the scaling invariant ratio

$$\eta_{\text{latt}} = \frac{g_x - 1}{|g_z|^{\frac{D-\Delta_\epsilon}{D-\Delta_\sigma}}} = \frac{g_x - 1}{|g_z|^{8/15}} \quad (6)$$

held fixed. The second equality uses the spacetime dimension $D = 2$ and scaling dimensions of the relevant Conformal field theory deformations $\Delta_\epsilon = 1$ and $\Delta_\sigma = 1/8$. For generic values of η_{latt} , the field theory describes massive interacting particles and is non-integrable. The lattice spacing is set to 1 throughout this work and all lengths are expressed in lattice units. The Hamiltonian $\hat{H}$ is dimensionless; hence, time is also dimensionless, and the operator $e^{-i\hat{H}t}$ describes evolution for dimensionless time t . More information on Ising field theory can be found in refs. 80–82.

Dynamical simulations of scattering in Ising field theory were recently performed using MPS methods in ref. 82. By changing the energy of the initial state, clear distinctions between elastic scattering, scattering near a resonance and particle production via inelastic scattering were observed. This work showcased the wealth of information that can be accessed with real-time simulations of collisions.

Our quantum simulations use $g_x = 1.25$ and $g_z = 0.15$ where there are two stable particles: one light particle $|1\rangle$ with mass $m_1 = 1.59$ and one heavy particle $|2\rangle$ with mass $m_2 = 2.98$. The initial state for our scattering simulations consists of two wavepackets of $|1\rangle$ particles that are separated in space. As time goes on, they travel towards each other, collide and separate. For low centre-of-mass energies E_{tot} , only the elastic process $11 \rightarrow 11$ shown in Fig. 2, left, is kinematically allowed. The lowest-energy inelastic process is $11 \rightarrow 12$ where a single heavy $|2\rangle$ particle is produced during the collision. The observation of this process is the goal of our quantum simulations. This inelastic channel opens

up for energies above the particle production threshold, $E_{\text{tot}} > E_{\text{thr}} = m_1 + m_2 = 4.57$ and can be detected from additional outgoing tracks in the energy density. This is seen in Fig. 2, right, which depicts the production of the heavy $|2\rangle$ particle. In the kinematic regime illustrated by Fig. 2, right, three different scattering outcomes occur in superposition: elastic scattering, inelastic scattering with the heavier particle moving right and inelastic scattering with the heavier particle moving left. Hence four outgoing tracks are visible, even though there are only two outgoing particles for each outcome.

For energies $E_{\text{tot}} \gg E_{\text{thr}}$ there are additional inelastic processes that produce many particles. Such processes generate substantial entanglement and are challenging to simulate with MPS methods. Simulations of these ultrahigh-energy collisions are also beyond the capabilities of current quantum hardware. At the energies accessed in our quantum simulations all inelastic channels besides $11 \rightarrow 12$ can be neglected. The three-body channel $11 \rightarrow 111$ is kinematically allowed but has a much smaller branching ratio than the $11 \rightarrow 12$ channel⁸² (see Supplementary Section C for details).

Inelastic scattering on IBM's quantum computers

In this section, inelastic scattering is simulated on $L = 104$ qubits of `ibm_marrakesh` using the lattice-to-qubit mapping shown in Fig. 3a. A lattice with open boundary conditions (OBCs) is chosen to avoid noisy gates. The boundary has exponentially small effects on wavepackets created in the bulk but causes the wavefunction to deviate from the ground state near the lattice edges. See ‘Details on the simulations performed using IBM’s quantum computers’ section in the Methods for a discussion, along with the modifications to the simulation protocols that are necessary to accommodate OBCs. The first step of the wavepacket preparation algorithm outlined in ‘Overview of the wavepacket preparation algorithm’ is the initialization of $|W(k_0)\rangle$. The ‘A constant-depth circuit for initializing $|W(k_0)\rangle$ ’ section in the Methods shows that this can be achieved with a constant-depth circuit using MCM-FF. This approach is currently not optimal on IBM’s `sheron r2` quantum computers due, in part, to readout being about $3\times$ noisier and $38\times$ slower than two-qubit gates (2,584 ns versus 68 ns). Instead of MCM-FF, $|W(k_0)\rangle$ is initialized with the unitary circuit in Extended Data Fig. 1, upper left. Wavepackets are then prepared by applying symmetry-preserving circuits $\hat{U}(\theta_*)$ that minimize the energy. These circuits are determined using ADAPT-VQE running on the MPS circuit simulator Quimb⁸³. Information on wavepacket preparation is given in the ‘Quantum circuits for preparing wavepackets in one-dimensional Ising field theory’ and ‘Quantum circuits for simulating scattering in one-dimensional Ising field theory’ sections in the Methods. The structure of the circuit that prepares two wavepackets is shown in Fig. 3b. The initial state is chosen so the wavepackets have

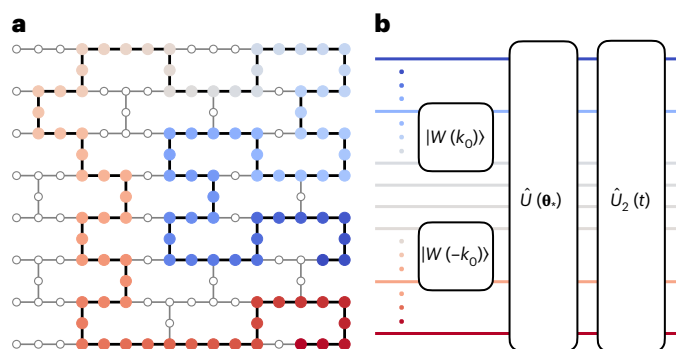


Fig. 3 | Qubit layout and circuit structure used to simulate scattering in Ising field theory. **a**, The $L = 104$ qubit layout used on `ibm_marrakesh`. **b**, The structure of the quantum circuits used to simulate scattering in Ising field theory. The colours indicate the qubits used in the lattice-to-device mapping. The energy minimization circuit $\hat{U}(\theta_*)$ creates wavepackets when acting on $|W(\pm k_0)\rangle$. The circuit $\hat{U}_2(t)$ implements time evolution with second-order Trotterization.

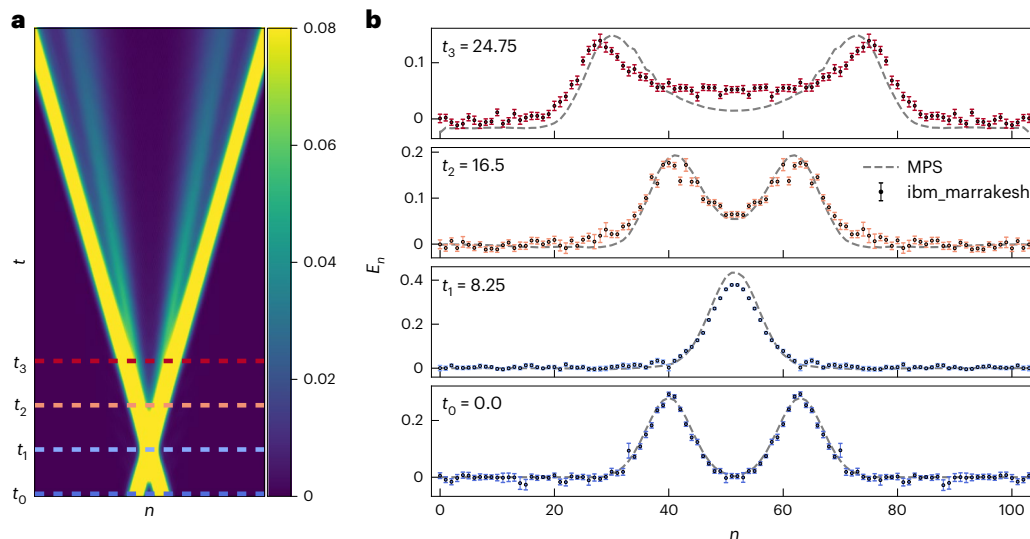


Fig. 4 | Simulations of inelastic particle production in one-dimensional Ising field theory. **a**, The energy density E_n throughout the scattering process obtained with a MPS circuit simulator on a $L = 256$ lattice. **b**, Results from simulations of scattering using $L = 104$ qubits of *ibm_marrakesh* for a selection of times depicted in **a**. The wavepackets are initialized at $t_0 = 0$ and collide around $t_1 = 8.25$. Outgoing particles begin to form at $t_2 = 16.5$ and $t_3 = 24.75$. The asymmetry of the energy density in each ‘bump’ signals the formation of the $|2\rangle$ particle

produced in the inelastic process $11 \rightarrow 12$. The y-axis range at each time is different to clearly show the features of the energy density. The initial wavepacket parameters are $k_0 = 0.32\pi$ and $\sigma = 0.13$, and each wavepacket is supported on $d \gtrsim 21$ sites. A Trotter step size of $\delta t = 1/16$ is used to evolve the system in **a** and $\delta t = 0.55$ is used in **b**. The sample size for **b** is (from bottom to top) $\{2.56, 1.28, 1.28, 2.56\} \times 10^6$, and the statistical error bars are the bootstrap standard error centred around the mean.

support on $d \gtrsim 21$ sites, and the total energy is $E_{\text{tot}}/E_{\text{thr}} = 1.2$. These parameters give the strongest signal of inelastic scattering in the least circuit depth (‘Details on the simulations performed using IBM’s quantum computers’ section in the Methods).

Once established, the wavepackets are time evolved with a second-order Trotterized unitary $\hat{U}_2(t)$. A Trotter step size of $\delta t = 0.55$ is chosen to balance the Trotter error and circuit depth (Supplementary Section G). For each simulation time, the vacuum-subtracted energy density

$$E_n = \langle \psi_{\text{2wp}} | \hat{H}_n(t) | \psi_{\text{2wp}} \rangle - \langle \psi_{\text{vac}} | \hat{H}_n(t) | \psi_{\text{vac}} \rangle \quad (7)$$

is measured. Here, $\hat{H}_n(t) = \hat{U}_2(t)^\dagger \hat{H}_n \hat{U}_2(t)$ with $\hat{H}_n$ defined in equation (5), $|\psi_{\text{2wp}}\rangle$ is the prepared two-wavepacket state and $|\psi_{\text{vac}}\rangle$ is the prepared vacuum. The circuits that prepare $|\psi_{\text{2wp}}\rangle$ and $|\psi_{\text{vac}}\rangle$ have very similar structure and are explained in the ‘Details on the simulations performed using IBM’s quantum computers’ section in the Methods.

MPS calculations of the energy density throughout the scattering process are shown in Fig. 4a. Two pairs of particle tracks emerge from the collision region. The majority of the energy is in the outer pair of tracks, which correspond to the trajectories of the light $|1\rangle$ particles. The inner pair of tracks has a lower velocity compared to the elastic trajectories and represent the heavy $|2\rangle$ particles produced in the inelastic process $11 \rightarrow 12$. Schematically, this process is

$$|1(k_0)1(-k_0)\rangle \rightarrow |1(k')2(-k')\rangle + 1 \leftrightarrow 2, \quad (8)$$

where k' is the momentum of outgoing particles. The kinematics are such that the trajectories of the outgoing $|1\rangle$ particles overlap with the elastic tracks and cannot be distinguished in Fig. 4a (see ‘MPS simulations of scattering in one-dimensional Ising field theory’ section in the Methods for details). It is shown in Supplementary Section C that the identification of the outgoing tracks with $|1\rangle$ and $|2\rangle$ particles is consistent with their velocities predicted from the single-particle dispersion relations. We emphasize that the elastic and inelastic processes occur in superposition, and there are no components of the wavefunction with four particles.

The energy density measured on *ibm_marrakesh* is shown for a selection of simulation times in Fig. 4b. Two distinct wavepackets initialized at $t_0 = 0$ propagate towards each other and collide around $t_1 = 8.25$. Later simulation times probe the formation and evolution of the post-collision state. At $t_2 = 16.5$ the outgoing wavepackets begin to separate, and by $t_3 = 24.75$, asymptotic particles begin to form. Up to $t_2 = 16.5$, there is good agreement between the energy density determined from *ibm_marrakesh* (data) and MPS (dashed grey line). Significant systematic errors develop in the quantum data at $t_3 = 24.75$ due to the larger circuit volume. For $t > t_3$, the asymptotic $|2\rangle$ particle produced in the $11 \rightarrow 12$ process becomes identifiable as a separate ‘bump’ in the energy density that propagates at a lower velocity. Unfortunately, the cumulative effects of noise made simulations beyond $t = 24.75$ impossible on *ibm_marrakesh*.

Despite the device noise, we observe evidence for the inelastic production of the heavy $|2\rangle$ particle. Long after the collision, the presence of a heavy particle could be confirmed by projecting onto exclusive scattering channels. Before this, the energy density of the outgoing particles on each side of the collision becomes skewed towards the centre of the lattice. This is due to the presence of the $|2\rangle$ particle in the wavefunction that travels slower and is absent for scattering below inelastic threshold, as shown in the ‘Calculating skewness’ section in the Methods. We compute the skewness, γ , from the third moment of the energy density of each region of outgoing particles as described in the ‘Calculating skewness’ section in the Methods. The left column of Fig. 5 shows the energy density of the bumps after the collision, and gives γ obtained from both MPS and *ibm_marrakesh*. The quantum results of the post-collision state at t_2 are right-skewed ($\gamma > 0$) and in agreement with MPS. The right-skewness increases at t_3 due to the emergence of the heavy $|2\rangle$ particle. Some of this skewness is due to systematic errors in the quantum data that increase E_n between the outgoing particles. To isolate skewness due to inelastic effects from systematic errors, additional simulations of single wavepacket propagation are performed. The energy density of a single wavepacket at times t_2 and t_3 are shown in the right column of Fig. 5. The MPS simulations of single wavepacket propagation still exhibit positive skewness due to boundary effects as discussed in the ‘Calculating skewness’

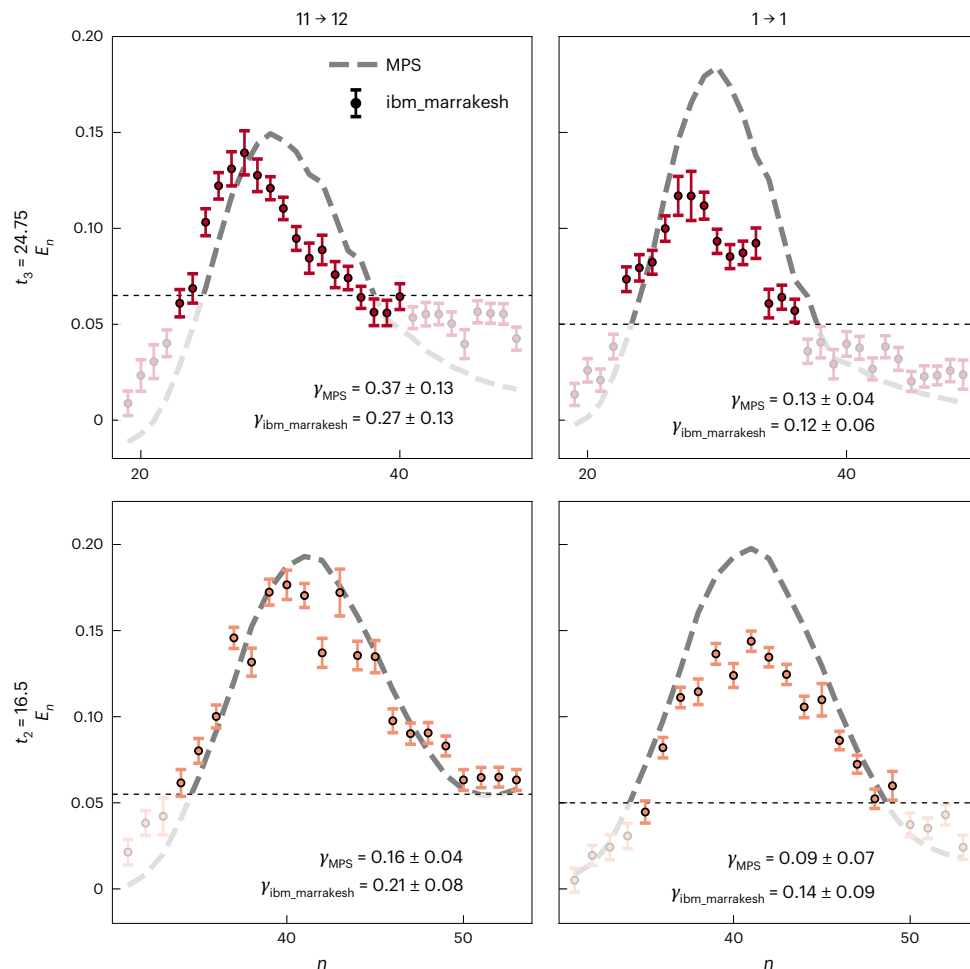


Fig. 5 | Asymmetry in the post-collision and single-particle energy densities.

The regions of positive energy density on the left half of the lattice in the $11 \rightarrow 12$ scattering process (left column) and in the $1 \rightarrow 1$ process of single particle propagation (right column). Results at times t_2 and t_3 obtained from *ibm_marrakesh* and MPS are shown. The skewness of the energy density, γ , is computed by considering points in an interval determined by an energy cutoff (dotted black line). The uncertainty in γ comes from varying the energy cutoff as

described in the ‘Calculating skewness’ section in the Methods and from statistical error. The skewness is increased in the $11 \rightarrow 12$ energy density compared to $1 \rightarrow 1$ due to the inelastic production of the heavy $|2\rangle$ particle. The simulation parameters are the same as in Fig. 4b. The sample size for the left column is (from bottom to top) $\{1.28, 2.56\} \times 10^6$ and for the right column is $\{2.56, 5.12\} \times 10^6$. The statistical error bars are the bootstrap standard error centred around the mean.

section in the Methods. The skewness of the post-collision state is 0.6σ larger than the single-particle state at t_2 and 1σ larger at t_3 . This provides evidence that the post-collision skewness is, at least partially, due to inelastic particle production.

The quantum resources used for these simulations are detailed in the ‘Error mitigation’ section in the Methods. The latest simulation time corresponds to $n_T = 45$ Trotter steps and requires 5,589 two-qubit gates with a two-qubit gate depth of 130. With such a large quantum volume, effective error mitigation is crucial for recovering reliable results. A full description of our error mitigation strategy is provided in the ‘Error mitigation’ section in the Methods, with certain aspects highlighted here. Pauli twirling (PT)⁸⁴ shapes the noise into a stochastic Pauli channel. For each simulation time, circuits that evolve both $|\psi_{\text{wp}}\rangle$ and $|\psi_{\text{vac}}\rangle$ are run. The time evolution of the vacuum is used to learn how the Pauli noise channel affects local observables. Noise-free expectation values in the scattering simulations are then estimated using the learned noise model. This method, known as operator decoherence renormalization (ODR)⁴⁶, is an extension of refs. 26,85.

Two unforeseen features of the device noise were encountered during the simulations. First, the Pauli noise channel is very asymmetric, and $\langle \hat{Z}_n \rangle$ measurements are effectively $\approx 3\times$ noisier than $\langle \hat{X}_n \rangle$ and $\langle \hat{Z}_n \hat{Z}_{n+1} \rangle$ measurements (see the ‘Error mitigation’ section in the Meth-

ods for details on device noise characteristics). The source of this asymmetry is a mystery but could be due to incomplete twirling of the (non-Clifford) R_{ZZ} gate. In addition, we observed that one faulty single- or two-qubit gate could degrade the whole simulation. This was not noticed in previous simulations of wavepacket dynamics on IBM’s quantum computers performed by the authors that utilized similar circuit depths^{47,48}. We attribute this increased sensitivity to the larger simulation light cone of $ct_{\text{max}} \approx 40$ qubits reached in this work, compared with $ct_{\text{max}} \approx 8$ qubits in our previous works. This effectively allows the noise to contaminate a larger region of the device in the same circuit depth. To reduce these effects, IBM’s calibration data was used to carefully avoid high-error gates in the lattice-to-qubit mapping. The simulation light-cone also explains the increase in systematic errors at t_3 compared with t_2 , despite the circuit depth only increasing by 30. This is because the simulation light-cone at t_3 encapsulates approximately $2.5\times$ more two-qubit gates than at t_2 . These observations highlight that the effects of circuit noise on the results of a quantum simulation depend heavily on the physical process being simulated.

Discussion

The quantum simulations in this work are the first to probe the non-equilibrium QFT dynamics generated in the wake of particle

collisions. This is a substantial improvement over previous quantum simulations of scattering that were constrained to early times and low energies. Advancing beyond this regime required sophisticated strategies for managing device errors that are amplified by a large simulation light cone ct_{max} . Algorithmic errors and quantum resource requirements must be balanced in an optimal simulation that operates within the correct regime of length scales. Our simulations of Ising field theory used: system size $L = 104$, particle propagation distance $vt_{\text{max}} \approx 40$, wavepacket size $d \approx 21$ and correlation length $\xi \approx 1/m \approx 0.6$ (where m is the mass of the lightest particle). Even with these minimal parameters, observing evidence of inelastic particle production required the full capability of state-of-the-art quantum hardware.

Our simulations are far from the continuum limit of $\xi \rightarrow \infty$ (in lattice units) and are not designed to make precise predictions about the underlying QFT. Instead, our work demonstrates that simulations far from the continuum can still be informative and capture features of non-equilibrium processes in QFTs. The use of quantum computers to explore quantum many-body dynamics, without the goal of making precise quantitative predictions, aligns with the capabilities expected in the pre-fault-tolerant era. Precision simulations of scattering are possible in one-dimensional QFTs using MPS techniques^{82,86–94}. For example, the Ising field theory simulations in ref. 82 utilized an L , vt_{max} , d , ξ and inverse time step $1/\delta t$ that were about $10\times$ larger than are used in this work. The smaller systematic errors in their simulations allowed individual inelastic channels to be isolated and enabled robust predictions of the underlying QFT. Future quantum simulations, probably incorporating some form of error correction, may be able to access ultrahigh-energy scattering where the production of highly entangled, many-particle states renders MPS methods unreliable.

The wavepacket preparation algorithm developed in this work is particularly advantageous in higher dimensions. By utilizing MCM-FF, wavepackets in any finite spatial dimension can be prepared with a circuit depth that is independent of the wavepacket size, provided that the qubits share the connectivity of the target lattice. By contrast, existing methods have a circuit depth that scales polynomially in the spatial volume of the wavepacket. This scaling is often worse if all-to-all connectivity is not assumed. The speedup from using MCM-FF arises because some long-range correlations in quantum states can be built with constant-depth circuits that are supplemented with local operations and classical communication. Efficient algorithms allocate the minimal amount of two-qubit gates needed to create the requisite entanglement, which is then distributed throughout the system with MCM-FF. The key insight is that the long-range entanglement inherent to momentum plane waves⁷⁵ is also present in W states⁹⁵. Therefore, wavepackets can be built from W states by only modifying correlations localized over $\approx \xi$ sites. Finding a basis where this observation is useful was guided by the symmetries and hierarchies in length scales characteristic of the target system.

The efficient preparation of wavepackets is a prerequisite for achieving a quantum advantage in simulations of scattering. An advantage could be realized in two dimensions, where no dynamical simulations of QFT scattering have ever been performed. The underlying assumption of classical hardness is supported by empirical evidence that simulations of dynamics in two dimensions are challenging using classical computers^{96–99}. Such simulations would unlock the ab initio study of many phenomena absent in one-dimensional systems. For example, in two dimensions, spatial rotations on the circle allow single particles to have spin, pairs of particles to have anyonic statistics, and multiple particles to have relative orbital angular momentum. Dynamical studies of these effects in QFTs are now possible^{100–104} due to the emergence of flagship quantum computers with native two-dimensional connectivity^{105–110}. These advancements have the potential to open a new frontier of scientific exploration that is powered by quantum computing.

Online content

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Methods

Throughout this Article, the qubits are labelled $|q_{L-1} \dots q_2 q_1 q_0\rangle$ (little-endian notation) and the top wire in every circuit corresponds to q_0 . The system size is L and all systems have PBCs (with $q_L = q_0$) unless otherwise stated. The wavepacket size is d , the mass of the lightest particle is m , $|\psi_{\text{wp}}\rangle$ is the exact wavepacket, $|\psi_{\text{ansatz}}\rangle$ is the approximately prepared wavepacket and $|\psi_{\text{vac}}\rangle$ is the vacuum.

A constant-depth circuit for initializing $|W(k_0)\rangle$

The efficient preparation of the state in equation (4) on d sites

$$|W(k_0)\rangle = \sum_{n=0}^{d-1} e^{i\phi_n} c_n |2^n\rangle, \quad (9)$$

is an important primitive for the preparation of wavepackets. For $\phi_n = 0$ and $c_n = 1/\sqrt{d}$ this reduces to the W state. The authors of ref. 64 presented an ingenious circuit for preparing the W state in constant depth that requires d ancilla qubits. Their method begins by initializing $|\psi_0\rangle = (\sqrt{1-\delta/d}|0\rangle + \sqrt{\delta/d}|1\rangle)^{\otimes d}$ on the system qubits. Then the parity $\prod \hat{Z}_n$ is measured using a constant-depth circuit. Odd parity occurs with $p_{\text{success}} \geq 0.43\delta$ and prepares the W state with infidelity $\mathcal{I} = \mathcal{O}(\delta^2)$. We generalize their method to prepare $|W(k_0)\rangle$ for arbitrary c_n and ϕ_n . In addition, we remove the ancillas and provide exact expressions for p_{success} and $\mathcal{I}$.

The circuit that prepares $|W(k_0)\rangle$ is shown in Extended Data Fig. 2. The states $|\psi_0\rangle$, $|\psi_1\rangle$, $|\psi_2\rangle$ are labelled at intermediate stages of the circuit and are described here. First, q_0 is prepared in $|+\rangle$ and

$$|\psi_0\rangle = \bigotimes_{n=0}^{d/2-1} \left[\cos\left(\frac{\theta_{2n+1}}{2}\right)|0\rangle + \sin\left(\frac{\theta_{2n+1}}{2}\right)|1\rangle \right], \quad (10)$$

$$\sin\left(\frac{\theta_{2n+1}}{2}\right) = \sqrt{\delta} \sqrt{c_{2n}^2 + c_{2n+1}^2},$$

is prepared on the odd-numbered qubits by applying single-qubit R_y rotations, $\prod_n e^{-i\theta_{2n+1}\hat{Y}_{2n+1}/2}$. Then, the parity is kicked back to qubit q_0 by applying $\prod_{n=0}^{d/2-1} \hat{Z}_{2n+1}$ controlled on q_0 . This controlled-parity operation is implemented with the constant-depth circuit developed in ref. 64 and shown in Extended Data Fig. 2, right. Several details about this circuit are described here. The second layer of CNOTs acts on pairs of qubits $q_n q_{n+2}$ with $n = 0, 4, \dots, d-6$. The p_n in the first round of MCM-FF are the sums of the outcomes on all measured qubits q_m with $m < n$, and the p in the second round of MCM-FF is the sum of all measurement outcomes. After applying the controlled $\prod_{n=0}^{d/2-1} \hat{Z}_{2n+1}$ and a Hadamard on qubit q_0 , the state of q_0 is correlated with the parity, that is, $|\psi\rangle = |\text{even parity}\rangle|0\rangle + |\text{odd parity}\rangle|1\rangle$.

Next, q_0 is measured and outcomes are post-selected on odd parity, which occurs with success probability

$$p_{\text{success}} = \frac{1}{2} - \frac{1}{2} \prod_{n=0}^{d/2-1} [1 - 2\delta(c_{2n}^2 + c_{2n+1}^2)]$$

$$= \delta - \delta^2 \left[1 - \sum_{n=0}^{d/2-1} (c_{2n}^2 + c_{2n+1}^2)^2 \right]$$

$$+ \frac{2}{3} \delta^3 \left[1 - 3 \sum_{n=0}^{d/2-1} (c_{2n}^2 + c_{2n+1}^2)^2 + 2 \sum_{n=0}^{d/2-1} (c_{2n}^2 + c_{2n+1}^2)^3 \right]$$

$$+ \mathcal{O}(\delta^4) \geq \frac{1}{2} (1 - e^{-2\delta}) \geq 0.43\delta. \quad (11)$$

This expression has been simplified by using the normalization condition $\sum_n c_n^2 = 1$. The lower bound of p_{success} is derived in Supplementary Section A for $\delta \leq 1$. The even-numbered qubits are reset to $|0\rangle$ and the state after a successful measurement outcome is

$$|\psi_1\rangle = \sum_{n=0}^{d/2-1} \sqrt{c_{2n}^2 + c_{2n+1}^2} |2^{n+1}\rangle + \mathcal{O}(\delta). \quad (12)$$

For a given pair of neighbouring qubits, this state has concentrated the probability of finding either in $|1\rangle$ to the odd-numbered qubits. Inspired by ref. 68, the final step spreads this probability to the even sites, previously used as ancillas. This is done using the controlled- R_y CNOT sequence from ref. 69, with rotation angles

$$\tan\left(\frac{\theta_{2n}}{2}\right) = \frac{c_{2n}}{c_{2n+1}}. \quad (13)$$

Lastly, the phases in $|W(k_0)\rangle$ are added with single-qubit R_z rotations, $\prod_n e^{-i\phi_n \hat{Z}_n/2}$. The final state $|\psi_2\rangle$ is an approximation to $|W(k_0)\rangle$ with infidelity

$$\mathcal{I} = 1 - |\langle W(k_0) | \psi_2 \rangle|^2$$

$$= 1 - \frac{1}{p_{\text{success}}} \sum_{n=0}^{d/2-1} \delta(c_{2n}^2 + c_{2n+1}^2) \prod_{\ell \neq n} [1 - \delta(c_{2\ell}^2 + c_{2\ell+1}^2)]$$

$$= \frac{\delta^2}{6} \left[1 - 3 \sum_{n=0}^{d/2-1} (c_{2n}^2 + c_{2n+1}^2)^2 + 2 \sum_{n=0}^{d/2-1} (c_{2n}^2 + c_{2n+1}^2)^3 \right]$$

$$+ \mathcal{O}(\delta^3) \leq \frac{\delta^2 (d-2)(d-4)}{6d^2} + \mathcal{O}(\delta^3). \quad (14)$$

The upper bound on $\mathcal{I}$ is derived in Supplementary Section A. Note that expanding $\mathcal{I}$ to the first non-zero order required p_{success} in equation (11) to third order. Both p_{success} and $\mathcal{I}$ are independent of d for large d , and their worst case bounds are saturated for W states.

Quantum circuits for preparing wavepackets in one-dimensional Ising field theory

The algorithm outlined in ‘Overview of the wavepacket preparation algorithm’ can prepare wavepackets in a wide range of lattice QFTs. This section provides the circuits for wavepackets in one-dimensional Ising field theory, with additional applications to $\lambda\phi^4$ scalar field theory and the Schwinger model, as well as two-dimensional Ising field theory, given in Supplementary Section B. Circuits that prepare wavepackets on system sizes with ≤ 28 qubits are found using the `qiskit` statevector simulator¹¹¹, and the prepared state is benchmarked against the exact wavepacket determined from exact diagonalization. Our exact diagonalization methods are explained in Supplementary Section H. In the ‘MPS simulations of scattering in one-dimensional Ising field theory’ section, the circuits that prepare wavepackets in one-dimensional Ising field theory on a $L = 256$ lattice are determined using a MPS circuit simulator.

MCM-FF is inefficient on classical circuit simulators because each measurement outcome creates a new branch in the circuit that must be computed separately. In the worst case, this causes the simulation cost to scale exponentially with the number of measurements. Therefore, all simulations that use classical computing in this work initialize $|W(k_0)\rangle$ with the unitary circuit in Extended Data Fig. 1, top left. The wavepackets prepared in this section using statevector simulators have the wavepacket size d equal to the system size L . Additional circuits for preparing $|W(k_0)\rangle$ that reduce the circuit depth by utilizing beyond-linear connectivity and/or MCM-FF are given in Supplementary Section D. The approximate wavepacket is then prepared by variationally minimizing the energy using circuits that are translationally invariant, real and preserve the other system-specific symmetries. We perform this optimization using ADAPT-VQE, which provides an efficient framework for symmetry-aware optimization. ADAPT-VQE is a greedy algorithm that builds the structure of the ansatz circuits layer by layer. At each step in the algorithm, the circuit layer that is most effective at minimizing the energy is identified from a pool of symmetry-preserving parameterized circuits $\{\hat{U}(\theta)\}$. This circuit layer is appended to the ansatz circuit and the values of the variational parameters θ are optimized to minimize the energy. The key ingredient in ADAPT-VQE is the choice of circuit pool, or equivalently an operator

pool $\{\hat{O}\}$ from which the circuits are generated, that is, $\hat{U}_j(\theta) = e^{i\theta\hat{O}_j}$. Guided by symmetries, an operator pool inspired by the Lie algebra of the Hamiltonian will be used throughout this work. Operator pools inspired by the Hamiltonian algebra have previously been used to great success in refs. 46–49,112–114. A full description of ADAPT-VQE is given in Supplementary Section F.

In one-dimensional Ising field theory, one lattice site maps to one qubit and the initial state for preparing wavepackets is the $|W(k_0)\rangle$ in equation (9). A unitary circuit that prepares $|W(k_0)\rangle$ is shown in Extended Data Fig. 1, top left. This circuit is most efficient for odd wavepacket sizes d . The R_y angles are given by recursively solving the equations

$$\begin{aligned} \left[\sin\left(\frac{\theta_n}{2}\right)\right]^2 &= \sum_{i=n}^{d-1} c_i^2, \\ \cos\left(\frac{\theta_{n+j+1}}{2}\right) \prod_{i=0}^j \sin\left(\frac{\theta_{n+i}}{2}\right) &= c_{n+j}, \quad j \in [0, 1, \dots, \eta-1], \\ \cos\left(\frac{\theta_n}{2}\right) \cos\left(\frac{\theta_{n-j-1}}{2}\right) \prod_{i=2}^j \sin\left(\frac{\theta_{n-i}}{2}\right) &= c_{n-j}, \quad j \in [1, 2, \dots, \eta-1], \end{aligned} \quad (15)$$

where $\eta \equiv (d-1)/2$. The R_z rotation angles are the ϕ_n from equation (9). The circuit depth scales linearly with wavepacket size

$$\text{CNOT depth: } 2\lfloor d/2 \rfloor + 2, \quad (16)$$

and is probably optimal assuming linear connectivity and no MCM-FF.

The next step in the wavepacket preparation algorithm is to apply translationally invariant and real circuits that minimize the energy. This is achieved by using ADAPT-VQE to optimize parameterized circuits $\{e^{i\theta\hat{O}}\}$ constructed from a symmetry-preserving pool of operators $\{\hat{O}\}_{1d \text{ Ising}}$. Enforcing reality and hermiticity constrains all pool operators to be imaginary and anti-symmetric, and the union of all unique operators generated from $i\sum_n [\hat{H}, \hat{X}_n]$ and $i\sum_n [\hat{H}, [\hat{H}, \hat{X}_n]]$ is found to be effective

$$\begin{aligned} \{\hat{O}\}_{1d \text{ Ising}} &= \sum_{n=0}^{L-1} \{ \hat{Y}_n, \hat{Z}_n \hat{Y}_{n+1} \hat{Z}_{n+2}, (\hat{Y}_n \hat{Z}_{n+1} + \hat{Z}_n \hat{Y}_{n+1}), (\hat{Y}_n \hat{X}_{n+1} + \hat{X}_n \hat{Y}_{n+1}), \\ &\quad (\hat{Z}_n \hat{X}_{n+1} \hat{Y}_{n+2} + \hat{Y}_n \hat{X}_{n+1} \hat{Z}_{n+2}) \}. \end{aligned} \quad (17)$$

Circuits implementing unitary evolution generated by the operators in the pool are given in Extended Data Fig. 1, top right. The construction of the circuits is based on the results in ref. 115, and details can be found in Supplementary Section I. The CNOT depth corresponding to the unitary evolution with respect to each pool operator in equation (17) is $\{0, 4, 4, 4, 8\}$.

To assess the quality of the ADAPT-VQE-prepared wavepacket $|\psi_{\text{ansatz}}\rangle$, we compare it to the exact wavepacket $|\psi_{\text{wp}}\rangle$ by computing the deviation of the energy $(E_{\text{wp}} - E_{\text{ansatz}})/m$ in units of the mass gap m , and the infidelity $1 - |\langle \psi_{\text{wp}} | \psi_{\text{ansatz}} \rangle|^2$. Extended Data Fig. 1 shows these two quantities as functions of CNOT depth, obtained from up to 12 steps of ADAPT-VQE for $L = 28$ and $\sigma = 0.13$, $k_0 = 0.36\pi$. Results are shown for four sets of couplings that approach the field-theory limit of vanishing mass gap $\{(g_x, g_z, m)\} = \{(1.25, 0.15, 1.6), (1.18, 0.08, 1.1), (1.15, 0.05, 0.8), (1.08, 0.03, 0.7)\}$. The circuits are optimized to minimize the energy (left plot), which improves the overlap with the target wavepacket (right plot). An infidelity < 0.12 is reached by depth 16 for all couplings considered.

A plateau in the convergence is observed around the sixth step (depth 16) of ADAPT-VQE for all couplings except $g_x = 1.25$, $g_z = 0.15$. In Supplementary Section F, it is shown that these plateaus can be overcome by expanding the operator pool to include terms in the Lie algebra of the Hamiltonian that correspond to fifth- and seventh-order

commutators. In general, the convergence to the target wavepacket degrades with decreasing mass gap (increasing correlation length). This is expected as deeper circuits are generically needed to build out longer correlations. Recently, it has been demonstrated that variational quantum algorithms that utilize MCM-FF have a more favourable optimization landscape¹¹⁶ and are able to more efficiently prepare states with long-range correlations^{117–119}. This is an exciting direction where further improvements are expected. The sequence of operators and variational parameters corresponding to the eighth step of ADAPT-VQE in Extended Data Fig. 1 are given in Supplementary Section J.

Quantum circuits for simulating scattering in one-dimensional Ising field theory

To reduce finite-size effects, the system size L must be much larger than the spatial extent of the wavepackets σ^{-1} . Because of this, it is pragmatic to set amplitudes in the $|W(k_0)\rangle$ wavefunction below some threshold to zero (and then normalize the wavefunction). This defines a wavepacket size d that depends on σ but is independent of L . The initial state is of the form

$$|\psi_{\text{ansatz}}\rangle \approx |0\rangle^{\otimes(L-d)/2} \otimes |W(k_0)\rangle \otimes |0\rangle^{\otimes(L-d)/2}, \quad (18)$$

and has errors that can be exponentially suppressed by increasing d . A wavepacket size of $d = 21$ is shown to have negligible truncation errors for $\sigma = 0.13$ (Supplementary Section G) and will be used throughout this section. Roughly speaking, the ADAPT-VQE circuit $\hat{U}(\theta_\star)$ that minimizes the energy acts as

$$\hat{U}(\theta_\star) \left(|0\rangle^{\otimes(L-d)/2} \otimes |W(k_0)\rangle \otimes |0\rangle^{\otimes(L-d)/2} \right) \rightarrow (|\psi_{\text{vac}}\rangle \otimes |\psi_{\text{wp}}\rangle \otimes |\psi_{\text{vac}}\rangle). \quad (19)$$

This expression is only schematic, as the wavefunction on the RHS does not factorize between vacuum and wavepacket components. However, sufficiently far from the region where $|W(k_0)\rangle$ was constructed, local observables are indistinguishable from their vacuum expectation value. This is due to the exponential decay of correlations inherent to one-dimensional gapped systems¹²⁰. As a result, the vacuum can be approximately prepared from

$$\hat{U}(\theta_\star)|0\rangle^{\otimes L} \approx |\psi_{\text{vac}}\rangle. \quad (20)$$

In Supplementary Section F, it is shown that this approximately prepared vacuum is of even higher quality than the corresponding wavepacket. All results presented have the energy density of this approximate vacuum subtracted, as defined in equation (7). This includes the results from scattering simulations, which have the energy density of the time-evolved approximate vacuum subtracted.

The structure of the circuit that is used to simulate scattering in one-dimensional Ising field theory is shown in Extended Data Fig. 3a. First, two wavepackets are prepared with opposite momenta. This is done by initializing $|W(k_0)\rangle$ and $|W(-k_0)\rangle$ at the desired locations (light red) and then acting with the circuit that minimizes the energy, $\hat{U}(\theta_\star)$ (grey). Note that the $\hat{U}(\theta_\star)$ for preparing $|\psi_{\text{ansatz}}(k_0)\rangle$ works equally well for preparing $|\psi_{\text{ansatz}}(-k_0)\rangle$ because

$$|\psi_{\text{ansatz}}(-k_0)\rangle = (\hat{U}(\theta_\star)|W(k_0)\rangle)^* = \hat{U}(\theta_\star)|W(-k_0)\rangle. \quad (21)$$

The first equality follows from time-reversal symmetry, and the second equality follows from using real unitaries in ADAPT-VQE. Lastly, steps of second-order Trotterized time evolution are applied (blue).

MPS simulations of scattering in one-dimensional Ising field theory

In this section, the circuit elements in Extended Data Fig. 3a are used to simulate scattering in one-dimensional Ising field theory with MPS.

The simulation parameters are: $L = 256$, $\sigma = 0.13$, $d = 22$ and $g_x = 1.25$, $g_z = 0.15$, with corresponding mass gap $m = 1.59$ determined from finite-size extrapolations (Supplementary Section C). The circuits that minimize energy and prepare wavepackets are determined by implementing ADAPT-VQE on the Quimb MPS circuit simulator⁸³. It is important to set optimization bounds on the variational parameters so that the optimizer does not explore highly entangled states that are not well represented by MPS. Some of the MPS simulations are performed using CuPy¹²¹ for GPU acceleration. Due to the separation of length scales, $L \gg d$, special care must be taken with the energy minimization in ADAPT-VQE. When $L \gg d$, the majority of $|\psi_{\text{ansatz}}\rangle$ in equation (18) is $|00 \dots 0\rangle$, and ADAPT-VQE prioritizes circuits that locally prepare the highest-quality vacuum. We address this problem by instead minimizing the energy density summed across an interval that is a few correlation lengths larger than d . This instance of ADAPT-VQE minimizes the energy density over $28 = d + 6 \approx d + 10m^{-1}$ sites, and slight variations in the size of the interval have negligible effects.

In the ‘Quantum circuits for preparing wavepackets in one-dimensional Ising field theory’ section, the prepared wavepackets were benchmarked against the exact wavepacket for $L = 28$. As comparison with the exact wavepacket on a $L = 256$ lattice is not possible, the energy densities of wavepackets on $L = 256$ and $L = 28$ lattices are compared instead. Differences in the energy density of the exact wavepackets are expected to be small due to the exponential convergence of the single-particle spectrum with increasing system size (Supplementary Section C). The energy density of wavepackets with $k_0 = 0.36\pi$ prepared from eight steps of ADAPT-VQE, as well as the energy density of the exact $L = 28$ wavepacket are shown in Extended Data Fig. 3b. Extended Data Fig. 3b, inset, shows that the differences in the energy density between the two prepared wavepackets are $\Delta E_n < 10^{-3}$. This is strong evidence that the $L = 256$ and $L = 28$ wavepackets are of similar quality. In addition, the energy density of the approximate vacuum on $L = 256$ sites, prepared as in equation (20), agrees to 0.01% with the vacuum on $L = 28$. The prepared wavepackets at other momenta exhibit similar behaviour. Further verification of the ADAPT-VQE circuits obtained with MPS comes from comparing the variational parameters determined for $L = 28$ and $L = 256$, which agree to four decimal places. The variational parameters and operators that prepare all of the wavepackets used in this section are provided in Supplementary Section J.

A goal of our simulations is to observe a clear distinction between scattering at energies above and below inelastic threshold. There are two stable particles for $g_x = 1.25$, $g_z = 0.15$: $|1\rangle$ with mass $m_1 = m = 1.59$ and $|2\rangle$ with mass $m_2 = 2.98$. Away from E_s theory^{80,81}, a stable particle is defined to have a mass less than $2m_1$ so that decay is kinematically forbidden. The existence of two stable particles at $\eta_{\text{latt}} = \frac{(g_x - 1)}{|g_z|^{8/15}} \approx 0.69$ is consistent with ref. 82. The lowest-energy inelastic threshold corresponds to two $|1\rangle$ particles colliding and producing one $|1\rangle$ particle and one $|2\rangle$ particle, that is, the process $11 \rightarrow 12$. This threshold is at a centre-of-mass energy of $E_{\text{thr}} = m_1 + m_2$. The corresponding threshold momentum can be found from inverting the single-particle dispersion relation and solving $E(k_{\text{thr}}) = E_{\text{thr}}/2$. In Supplementary Section C, the dispersion relation is computed exactly for $L = \{16, 17, \dots, 28\}$ and shown to be exponentially converged in system size. The predicted threshold momentum is $|k_{\text{thr}}| \approx 0.24\pi$. However, since our wavepackets are obtained via variational energy minimization, their energy is strictly higher than that of the exact wavepacket. Because of this, the actual momentum threshold is a bit lower, closer to $|k_{\text{thr}}| \approx 0.22\pi$. Moreover, the inelastic threshold is not sharp due to the spread in momentum (or equivalently in energy) coming from a finite σ .

Results from MPS circuit simulations of scattering are shown in Extended Data Fig. 4. These simulations compute the vacuum-subtracted energy density E_n in equation (7) as a function of lattice position and simulation time. Each plot is labelled by the total energy E_{tot} and momentum k_0 of the wavepackets. The elastic process $11 \rightarrow 11$ is identified from

outgoing particles with the same velocity as the incoming particles. As shown schematically in Fig. 2, the inelastic process $11 \rightarrow 12$ converts some of the kinetic energy to mass to produce the heavier $|2\rangle$ particle. As a result, the outgoing particles travel slower than the incoming ones. The lowest momentum, $k_0 = 0.18\pi$, is well below inelastic threshold, and only elastic scattering is observed. Scattering at $k_0 = 0.2\pi$ reveals a very faint track in the middle of the lattice that does not propagate. This corresponds to $11 \rightarrow 12$ where the post-collision particles are at rest. Increasing the momentum further causes the left- and right-moving particle $|2\rangle$ tracks to be more identifiable, as shown in the plots for $k_0 \geq 0.28\pi$. The kinematics are such that the particle $|1\rangle$ tracks in $11 \rightarrow 12$ are hidden behind the elastic scattering trajectories. It is important to remember that expectations are averaged over the whole scattering wavefunction, which, in the case of $k_0 \leq 0.36\pi$, is a superposition of components with at most two particles. This discussion has ignored three-particle production that can occur for $E_{\text{tot}} > 3m_1 = 1.04E_{\text{thr}}$, as it has a much smaller branching ratio compared to $11 \rightarrow 12$ (ref. 82). See Supplementary Section C for a discussion of the other inelastic processes. The MPS simulations used a maximum bond dimension of $\text{max_bond} = 350$ and the energy density was converged to 0.01%.

Details on the simulations performed using IBM’s quantum computers

The simulations performed on IBM’s quantum computers in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ use parameters that are chosen to maximize the clarity of the inelastic effects in the results. The interplay between the parameters is nontrivial, and our simulation choices were informed by the following considerations:

- OBCs: OBCs are chosen instead of PBCs due to increased flexibility in the lattice-to-qubit mapping (see next point).
- $L = 104$: this was the largest lattice that could be mapped to `ibm_marrakesh` while maintaining a maximum CZ gate error of 7.5×10^{-3} .
- $\delta t = 0.55$: this was the largest Trotter step size that did not have notable Trotter errors. See Supplementary Section G for a quantification of the Trotter errors.
- $t_{\text{max}} = 24.75$ ($n_T = 45$ Trotter steps): this was the maximum simulation time that could be reached before the results were overwhelmed by device errors.
- $k_0 = 0.32\pi$: informed by the results of MPS scattering simulations shown in Extended Data Fig. 4, we determined that a wavepacket momentum of $k_0 = 0.32\pi$ has the strongest signal of inelastic scattering at $t_{\text{max}} = 24.75$.
- $\sigma = 0.13$: the wavepacket extent in momentum space was chosen to minimize the wavepacket’s spatial size and its spreading under time evolution. Wavepacket spreading is most significant for low-energy, elastic scattering, for example, $k_0 = 0.18\pi$ in Extended Data Fig. 4. Clearly resolving elastic and inelastic scattering, that is, distinguishing wavepacket delocalization and particle production, requires $\sigma \leq 0.13$. This is shown in Supplementary Section G.
- $d = 21$: this is the smallest spatial extent of $|W(k_0)\rangle$ that could be chosen for $\sigma = 0.13$ while keeping truncation effects small, see Supplementary Section G.
- No MCM-FF: the unitary $|W(k_0)\rangle$ preparation circuit in Extended Data Fig. 1, top left, was less noisy when run on `ibm_marrakesh` than the constant-depth circuit in Extended Data Fig. 2 that utilizes MCM-FF.
- Seven steps of ADAPT-VQE: the quality of the prepared wavepacket notably improves at seven steps.
- Two-site wavepacket separation: this is the smallest separation that keeps interactions between the initial wavepackets negligible and preserves the $E_n = E_{L-1-n}$ reflection symmetry.

The wavepacket preparation algorithm presented in this work relies on having a Hamiltonian that is block-diagonal in momentum space. This is a consequence of translational symmetry, which is broken in a system with OBCs. However, with OBCs, there is still an approximate translational symmetry in the bulk. For this reason, the quantum circuits that prepare PBC wavepackets can also be used to prepare wavepackets in a system with OBCs, if they act sufficiently far from the boundaries. The initial state of the quantum simulations in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ has wavepackets localized $\gtrsim 30$ sites from the boundary. This is much larger than the correlation length and therefore boundary effects may be ignored. The circuits that minimize the energy and prepare wavepackets are determined in a system with PBCs to preserve the momentum content established by $|W(k_0)\rangle$. The wavepacket with OBCs is prepared using the same circuit as for PBCs, but with all elements corresponding to Pauli strings that couple q_0, q_{L-1} removed. This causes the local vacuum near the boundaries to be of slightly lower quality than the rest of the state. Time evolution is then implemented with the OBC Ising field theory Hamiltonian, equation (5) without the $\hat{Z}_0\hat{Z}_{L-1}$ term.

The effects of OBCs on the quantum simulations in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ are illustrated in Extended Data Fig. 5. Extended Data Fig. 5, left, shows a MPS simulation of the energy density throughout the inelastic scattering process in a $L = 100$ system with OBCs. The quality of the vacuum near the boundaries is lower than in the bulk, causing small perturbations to propagate inwards. At $t \approx 20$, these perturbations interact with the post-collision state and generate small ripples in the energy density between the outgoing particles. This is shown in more detail in Extended Data Fig. 5, right, which compares the energy density in an OBC and PBC simulation. At $t = 20$ the energy density is nearly identical and there are almost no boundary effects. At $t = 30$, fluctuations coming from the boundaries can be identified in the energy density between the particles. These small fluctuations could be mitigated by adding boundary operators to the ADAPT-VQE operator pool to improve the vacuum near the edges⁴⁶.

The structure of the circuit that simulates scattering in Ising field theory is shown in Extended Data Fig. 3a. The initial state is prepared using the unitary circuit whose structure is shown in Extended Data Fig. 1, top left. The symmetry-preserving circuits that minimize the energy and prepare wavepackets are determined by implementing ADAPT-VQE with a MPS circuit simulator. This is described in the ‘MPS simulations of scattering in one-dimensional Ising field theory’ section, and the operator ordering and variational parameters that minimize the energy are given in Supplementary Section J. The corresponding circuits used in ADAPT-VQE are shown in Extended Data Fig. 1, top right. Time evolution is implemented using n_T second-order Trotter steps with ordering $\{R_x, R_z, R_{zz}, R_x\}$. The total circuit depth for the simulations is

$$\text{two-qubit gate depth: } 22 + 18 + 2n_T, \quad (22)$$

with the terms corresponding to the preparation of $|W(k_0)\rangle$ with $d = 21$, seven steps of ADAPT-VQE and n_T steps of Trotterized time evolution. The total circuit depth and number of two-qubit gates used in the quantum simulations are provided in Extended Data Table 1.

IBM’s *heron* quantum computers support fractional gates¹²², which include a native $R_{zz}(\theta) = e^{-i\theta ZZ/2}$ for $\theta \in [0, \pi/2)$. Trotterized time evolution requires $e^{i\delta t ZZ}$ with the opposite sign of θ . This could be overcome by sandwiching the R_{zz} gates with $\hat{X}$ to flip the sign of θ at the cost of two additional single-qubit gates per R_{zz} . To eliminate the single-qubit gate overhead, we instead swap the positions of the wavepackets and evolve backwards in time. Time reversal symmetry ensures that this simulates exactly the same scattering process. By using R_{zz} instead of CZ gates, the two-qubit gate depth of each Trotter step is reduced from 4 to 2. At the beginning of each run, we execute a

suite of R_{zz} calibration circuits to tune the rotation angles and reduce coherent errors.

At the end of the simulations, the energy density in equation (7) is measured and compared to the expected, noise-free, value obtained by simulating the same circuits with the Quimb MPS simulator. With OBCs, the energy density $\hat{H}_n$ in equation (5) on sites 0 and $L - 1$ contains only a single ZZ term without the $1/2$ prefactor. A relatively large $\delta t = 0.55$ causes the bond dimension to become quite large to maintain accuracy. Our MPS simulations required a bond dimension up to $\text{max_bond} = 2,250$ to be well converged at $t = 40$. Increasing the maximum bond dimension from 2,000 to 2,250 only changes the energy density by 8×10^{-4} . In comparison, $\text{max_bond} = 350$ was sufficient for the MPS scattering simulations shown in Extended Data Fig. 4 because they used a much smaller Trotter step size of $\delta t = 1/16$.

Error mitigation. A suite of error mitigation methods allows accurate predictions of observables to be made from noisy device data. Dynamical decoupling^{123,124} removes the effects of idle noise and crosstalk between qubits. PT⁸⁴ is applied to every two-qubit gate to convert coherent errors into stochastic noise. The 16 combinations of Paulis are used to twirl CZ gates, while the eight combinations given in Extended Data Fig. 6 are used for R_{zz} (a larger set compared with the one used in ref. 125). The complete Pauli basis for twirling $R_{zz}(\theta)$ is not available because it is a non-Clifford operation for arbitrary θ . Twirled readout error extinction (TREX)¹²⁶ is used to mitigate measurement errors. In the limit of infinite PT and TREX, the noise is characterized by a Pauli channel⁸⁴

$$\rho \rightarrow \sum_i p_i \hat{P}_i \rho \hat{P}_i, \quad (23)$$

where the sum runs over all 4^L Pauli operators $\hat{P}_i$ and $\sum_i p_i = 1$ with $p_i \geq 0$. Under this channel, expectation values of observables $\hat{O}$ are given by

$$\langle \hat{O} \rangle_{\text{meas}} = \sum_i p_i \text{Tr}(\hat{P}_i \rho \hat{P}_i \hat{O}). \quad (24)$$

For Pauli observables, $\hat{P}_i \hat{O} \hat{P}_i = \pm \hat{O}$, and this channel scales the measured values $\langle \hat{O} \rangle_{\text{meas}}$ relative to their predicted (noise-free) counterparts $\langle \hat{O} \rangle_{\text{pred}}$: $\langle \hat{O} \rangle_{\text{meas}} = p_{\hat{O}} \langle \hat{O} \rangle_{\text{pred}}$. The signal strength $|p_{\hat{O}}| \leq 1$ characterizes how much an observable is impacted by the Pauli noise channel.

Expectation values of local observables are then estimated using ODR^{26,46,47,85}. For each observable $\hat{O}$, the signal strength $p_{\hat{O}}$ is determined using a ‘mitigation’ circuit whose noise profile is similar to the original ‘physics’ circuit but whose output can be efficiently computed with classical computers. In this work, the Trotterized time evolution of the vacuum state, $\hat{U}_2(t)|\psi_{\text{vac}}\rangle$ is used for the mitigation circuit. With exact state preparation and time evolution, $e^{-i\hat{H}t}|\psi_{\text{vac}}\rangle$ is trivial since $|\psi_{\text{vac}}\rangle$ is an eigenstate of $\hat{H}$. In our simulations, errors coming from the approximate preparation of the vacuum in equation (20) are negligible. However, Trotter errors are large and cause the energy density to fluctuate up to 15% during time evolution (Supplementary Section G). These fluctuations can be mitigated by enforcing energy conservation in post-processing (see Supplementary Section K for more details).

The observables evaluated in the time-evolved (approximate) vacuum are calculated via MPS. For early times, this is efficient in one dimension due to the correspondence between ground states of gapped systems and area law entanglement¹²⁷. The signal strength is computed from the mitigation circuit results,

$$p_{\hat{O}} = \frac{\langle \hat{O} \rangle_{\text{meas}}}{\langle \hat{O} \rangle_{\text{pred}}} = \frac{\langle \psi_{\text{vac}} | \hat{U}_2^\dagger(t) \hat{O} \hat{U}_2(t) | \psi_{\text{vac}} \rangle_{\text{meas}}}{\langle \psi_{\text{vac}} | \hat{U}_2^\dagger(t) \hat{O} \hat{U}_2(t) | \psi_{\text{vac}} \rangle_{\text{pred}}}. \quad (25)$$

This $p_{\hat{O}}$ is then used to rescale $\langle \hat{O} \rangle_{\text{meas}}$ in the physics circuit and estimate its noise-free value. The $p_{\hat{O}}$ are also able to identify device runs with anomalously large amounts of noise. We filter out observables with $p_{\hat{O}} < 0.01$ (ref. 47) and observables that involve a qubit with readout

error $\epsilon_{\text{readout}} > 0.035$. In addition, there is a parity symmetry that equates the energy density of sites that are related by reflection about the collision point. For our simulations this implies $E_n = E_{L-1-n}$. By combining the uncorrelated measurements of observables related by this symmetry, our number of shots is effectively doubled.

A total of 16 TREX twirls, each with 500 shots, is used to mitigate the measurement errors for every PT, and the number of PTs run for each of the physics and mitigation circuits is given in Extended Data Table 1. Moreover, measurements must be performed in both the X - and Z -bases to determine the energy density. For $t_3 = 24.75$, this gives a total of $500 \times 16 \times 80 \times 2 \times 2 = 2.56 \times 10^6$ shots. It is important that the PT and TREX twirls are applied identically for each pair of physics and mitigation circuits, so that their noise profiles are as similar as possible. The mitigation circuits also work for TREX calibration, and no additional circuits are needed to mitigate readout errors. The initial state used for mitigation, $|\psi_{\text{vac}}\rangle$, is prepared by acting the wavepacket ADAPT-VQE circuit on the $|000\dots\rangle$ state (see the discussion around equation (20)). It is desirable to have maximal similarity between the structure and noise profiles of the physics and mitigation circuits. This is accomplished by preparing $|000\dots\rangle$ with the $|W(k_0)\rangle$ circuit in Extended Data Fig. 3a, but with the angle of the first R_Y -gate set to zero and the second CNOT changed from a control on $|0\rangle$ to a control on $|1\rangle$. An average over TREX twirls is taken to compute an expectation value for each observable for each PT. This is then used as input to the rest of the error mitigation pipeline. The expectation values $\langle \hat{Z}_n \rangle$, $\langle \hat{X}_n \rangle$ and $\langle \hat{Z}_n \hat{Z}_{n+1} \rangle$ are computed separately then added together to form the energy density.

The raw and error-mitigated results are compared in Extended Data Fig. 7 for $t_3 = 24.75$. The raw data from the device is close to the limit of pure depolarizing noise, which is far from the expected values determined from MPS. The results after error mitigation are significantly improved and lie close to MPS expectations. There exist points in the bottom panel of Extended Data Fig. 7 where the device results disagree with the MPS expectations by several standard deviations, despite all error mitigation techniques. This is particularly noticeable in the regions containing the outgoing particles, highlighting a weakness of the chosen mitigation circuits for ODR. The time evolution of the vacuum used as the reference state in ODR, $U_2(t) |\psi_{\text{vac}}\rangle$, does not capture effects of state-dependent noise on the wavepackets.

The signal strengths for $\langle \hat{Z}_n \rangle$, $\langle \hat{X}_n \rangle$, and $\langle \hat{Z}_n \hat{Z}_{n+1} \rangle$ at $t_3 = 24.75$ are shown in Extended Data Fig. 7, top left. The signal strength for $\hat{Z}$ is consistently $\approx 3 \times$ lower than for the other observables. This indicates that the weights p_i in the Pauli noise channel equation (23) are larger for the Paulis that anticommute with $\hat{Z}_n$. The Extended Data Fig. 7, top right, shows both the raw and ODR-predicted estimates for the different observables at a single site $n = 40$. The extra noise in $\langle \hat{Z}_n \rangle$ leads to substantially larger variations in the ODR-predicted $\langle \hat{Z}_n \rangle$ across Pauli twirls compared to the other observables. These large variations are a major cause of uncertainty in the final results, shown in Extended Data Fig. 7, bottom. We additionally computed $\langle \hat{X}_n \hat{X}_{n+1} \rangle$ and found that it is as noisy as $\langle \hat{Z}_n \rangle$. More extensive simulations are needed to identify the origin of this asymmetry. One cause could be the incomplete twirling of the R_{ZZ} gate (only 8 combinations of the 16 are possible). Another could be the imbalance of the couplings $g_x = 1.25$, $g_z = 0.15$.

Calculating skewness

The inelastic process $11 \rightarrow 12$ probed by the quantum simulations presented in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ produces a heavy $|2\rangle$ particle that travels slower than the lighter $|1\rangle$ particle. At late times, the $|2\rangle$ particle can be identified as a distinct bump in the energy density that travels slower. Before this, but after the collision, the emergence of the heavy $|2\rangle$ particle skews the outgoing energy profile towards the point of the collision. This skewness was identified in the data presented in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ and is evidence for inelastic particle production.

Our metric for the skewness is designed to account for the discrete nature of the data and incorporate statistical errors and device noise. We compute the skewness of the energy density over an interval of sites $j \in [n_{\text{min}}, n_{\text{max}}]$ that captures the region of positive energy density on one half of the lattice (the energy density is symmetrized about the centre of the collision as a part of error mitigation; see the ‘Details on the simulations performed using IBM’s quantum computers’ section for details). Given an energy cutoff ϵ , the window $[n_{\text{min}}, n_{\text{max}}]$ is chosen by contiguously including sites where $E_n + \sigma_n \geq \epsilon$, where E_n and its standard deviation σ_n are computed via bootstrap resampling as detailed in the ‘Details on the simulations performed using IBM’s quantum computers’ section. The energy cutoffs are chosen to capture as much of the region of excitations as possible, while omitting outliers caused by noise. For each time, the energy cutoff is varied across a range given in Extended Data Table 2 to estimate systematic errors. For each ϵ , we compute the third moment γ_ϵ of the distribution of the energy density

$$\gamma_\epsilon = \frac{\sum_j (j - \mu)^3 \tilde{E}_j}{\sigma_\epsilon^3}, \quad (26)$$

where the normalized energy density $\tilde{E}$, mean μ and standard deviation σ_ϵ are defined as

$$\tilde{E}_n = \frac{E_n}{\sum_j E_j}, \quad \mu = \sum_j j \tilde{E}_j, \quad \sigma_\epsilon^2 = \sum_j (j - \mu)^2 \tilde{E}_j. \quad (27)$$

The sums run over all sites in the window $[n_{\text{min}}, n_{\text{max}}]$. The skewness metric γ reported in ‘Quantum simulations of scattering in one-dimensional Ising field theory’ is calculated from $\{\gamma_\epsilon\}$

$$\gamma = \frac{\max \gamma_\epsilon + \min \gamma_\epsilon}{2}. \quad (28)$$

A positive value of γ corresponds to a right-skewed distribution, while a negative γ corresponds to a left-skewed one. Considerable variations are observed in the γ_ϵ values computed from different ϵ . Reflecting this, the error bars for γ include both the statistical errors from bootstrap resampling γ_ϵ and the variation of γ_ϵ with the cutoff ϵ . Extended Data Fig. 8, top, shows an example of the choice of cutoffs for $t_2 = 16.5$, as well as the resulting values of γ_ϵ for each ϵ , and the reported values of γ along with the error bars.

Extended Data Fig. 8, bottom, compares the skewness in MPS simulations of elastic ($k_0 = 0.18\pi$) and inelastic ($k_0 = 0.32\pi$) scattering. Despite small fluctuations coming from the discrete nature of the data, a clear trend is identified distinguishing the elastic and inelastic channels. The skewness is consistent with 0 before the collision for both momenta. After the collision ($t \approx 12$ – 15), the skewness increases for inelastic scattering and stays close to zero for elastic scattering. This reinforces the use of skewness of the energy density as a quantitative metric to detect inelastic effects shortly after the collision. Extended Data Fig. 8a shows the skewness in a large system with PBCs and larger wavepackets, whereas Extended Data Fig. 8b replicates the simulations that were ran on ibm_marrakesh for Figs. 4 and 5. Differences between Extended Data Fig. 8a,b are primarily due to boundary effects and Trotter errors.

Data availability

The processed data supporting the experimental findings of this work are included in Supplementary Section L. The remaining raw datasets generated during this work are available from the corresponding author upon reasonable request.

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Author contributions

R.C.F. and J.P. conceived the research direction of simulating one-dimensional Ising field theory on a quantum computer. R.C.F. developed the wavepacket preparation algorithm, and R.C.F. and N.A.Z. performed classical simulations of the state preparation and scattering circuits to validate the approach. R.C.F., N.A.Z. and M.I. worked on the design of the quantum circuits, and R.C.F. and N.A.Z. carried out the experiments on IBM's quantum computers. All authors contributed to interpreting the experimental data and to writing the manuscript.

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Competing interests

J.P. is a shareholder and part-time employee of Oratomic, Inc., which is developing fault-tolerant quantum computers. The other authors declare no competing interests.

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Extended Data Table 1 | Resources used in the quantum simulations performed on 104 qubits of ibm_marrakesh

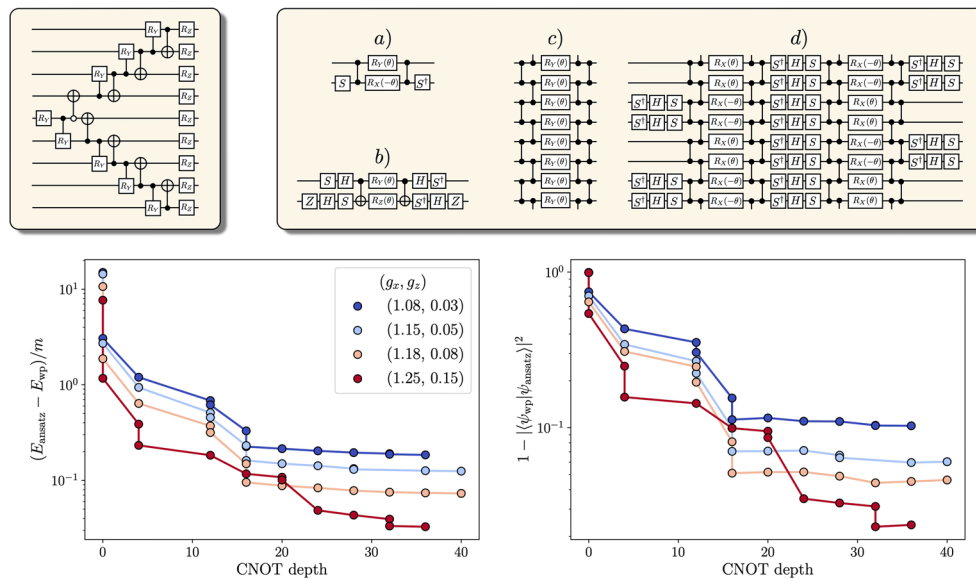
t	n_T	# of two-qubit gates	Two-qubit gate depth	# of PTs	# of shots
0	0	954	40	80	2.56×10^6
8.25	15	2,499	70	40	1.28×10^6
16.5	30	4,044 (4,022)	100	40 (80)	1.28×10^6 (2.56×10^6)
24.75	45	5,589 (5,567)	130	80 (160)	2.56×10^6 (5.12×10^6)

For a given simulation time t (first column), the number of Trotter steps n_T is given in the second column. The total number of two-qubit gates and corresponding two-qubit gate depth is given in columns three and four, respectively. The total number of Pauli twirls and shots per simulation time, including all error mitigation overhead, are given in columns five and six, respectively. The quantities in parentheses correspond to the single wavepacket simulations.

Extended Data Table 2 | The ranges of energy cutoffs, ϵ , used for calculating γ from the energy density obtained from MPS simulations and ibm_marrakesh

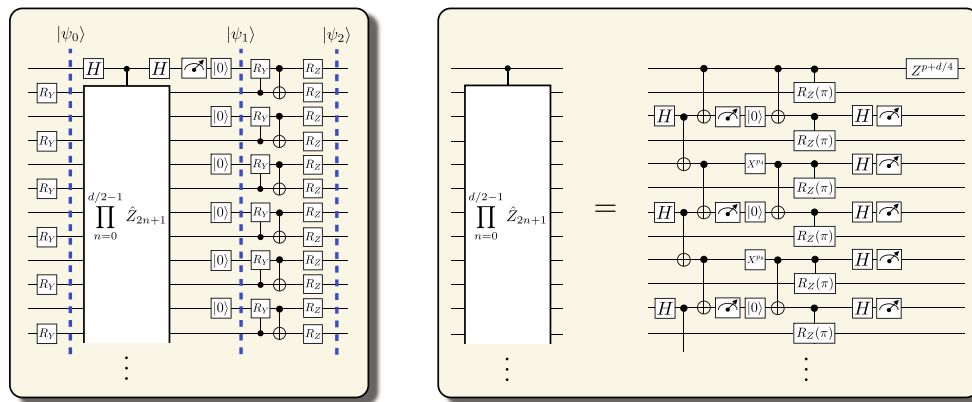
Initial state	t	ϵ_{MPS}	$\epsilon_{\text{ibm_marrakesh}}$	γ_{MPS}	$\gamma_{\text{ibm_marrakesh}}$
$ \psi_{2\text{wp}}\rangle$	24.75	0.02–0.04	0.065–0.085	0.37(13)	0.27(13)
$ \psi_{1\text{wp}}\rangle$	24.75	0.03–0.05	0.05–0.07	0.13(4)	0.12(6)
$ \psi_{2\text{wp}}\rangle$	16.5	0.055–0.075	0.055–0.075	0.16(4)	0.21(8)
$ \psi_{1\text{wp}}\rangle$	16.5	0.03–0.05	0.05–0.07	0.09(7)	0.14(9)
$ \psi_{2\text{wp}}\rangle$	0	0.02–0.04	0.02–0.04	0.0(0)	–0.09(7)

Cutoffs in increments of 0.005 are used.

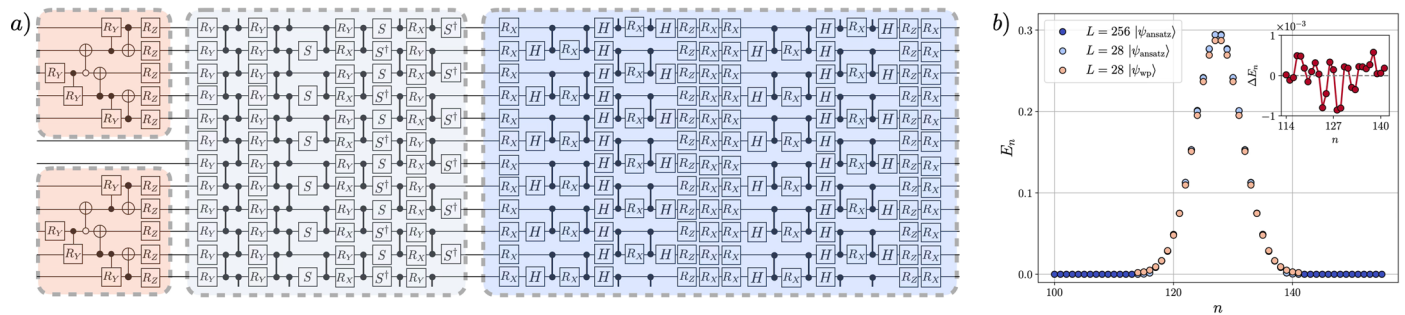


Extended Data Fig. 1 | Ising field theory preparation circuits and ADAPT-VQE performance. Upper: Circuits used to prepare wavepackets in one-dimensional Ising field theory. Left: a unitary circuit that prepares $|W(k_0)\rangle$ in Eq. 9 across 9 sites. The rotation angles are given in Eq. 15. Right: circuit elements used in ADAPT-VQE to prepare wavepackets in Ising field theory. They implement the unitary evolution of the operators in Eq. 17. **a)** implements $\exp[-i(\theta/2)(YZ + ZY)]$ and **b)** implements $\exp[-i(\theta/2)(YX + XY)]$. Examples of circuits that implement

$\exp[-i(\theta/2) \sum ZYZ]$ and $\exp[-i(\theta/2) \sum (ZXY + YXZ)]$ across 8 qubits with PBCs are shown in **c)** and **d)**, respectively. Lower: Quality of prepared wavepackets in one-dimensional Ising field theory. The deviation in energy (left) and infidelity (right) of the prepared wavepacket as a function of CNOT depth. The CNOT depth is monotonically related to the step of ADAPT-VQE, and corresponds to the additional depth after $|W(k_0)\rangle$ preparation. Results are shown for wavepacket parameters $\sigma = 0.13$, $k_0 = 0.367$ and $L = 28$ for various couplings g_x, g_z .

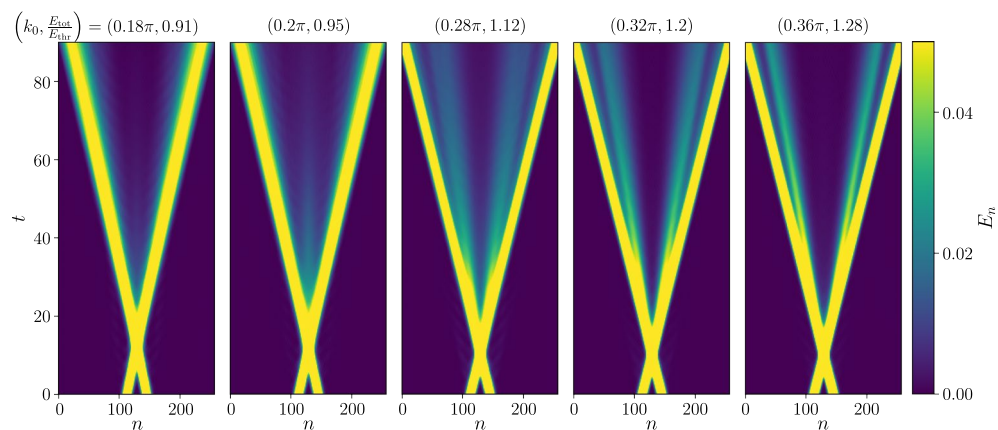


Extended Data Fig. 2 | Circuits that prepare $|W(k_0)\rangle$ in constant depth using MCM-FF. Left: a circuit that prepares $|W(k_0)\rangle$ in Eq. 9. Right: the circuit from ref. 64 that implements the global controlled unitary in constant depth.



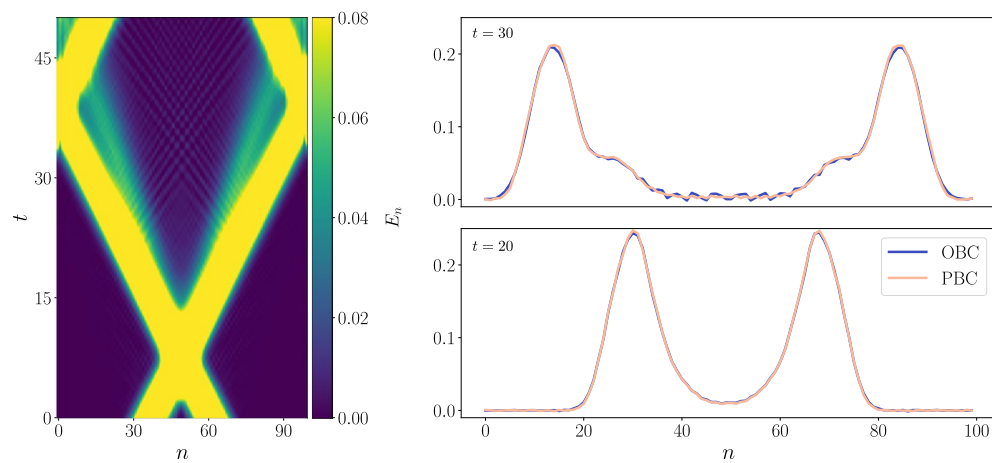
Extended Data Fig. 3 | Scattering circuits and wavepackets on large versus small lattices in one-dimensional Ising field theory. a) Circuits for simulating scattering in one-dimensional Ising field theory. A circuit that simulates the scattering of two $d=5$ wavepackets on a $L=12$ lattice. The pieces of the circuit highlighted in light red prepare $|W(k_0)\rangle$ and $|W(-k_0)\rangle$, the layer in gray represents the symmetry-preserving energy minimization circuit $U(\theta^*)$, and the layer in blue is two steps of second-order Trotterized time evolution $U_2(t)$. **b)** Comparison of wavepackets prepared on large and small lattices in one-dimensional Ising field

theory. The vacuum-subtracted energy density E_n of a wavepacket with $g_x = 1.25$, $g_z = 0.15$, $k_0 = 0.36\pi$, $\sigma = 0.13$ and $d=22$. The approximate wavepackets $|\psi_{\text{ansatz}}\rangle$ are prepared from 8 steps of ADAPT-VQE on a $L=256$ lattice (dark blue) and a $L=28$ lattice (light blue). The energy density of the exact $L=28$ wavepacket is also shown (tan). The inset shows the difference in the energy density ΔE_n between the approximate $L=28$ and $L=256$ wavepackets. Only the energy density of the 56 sites in the center of the lattice is shown, and the $L=28$ wavepackets are translated to align with the $L=256$ wavepacket.



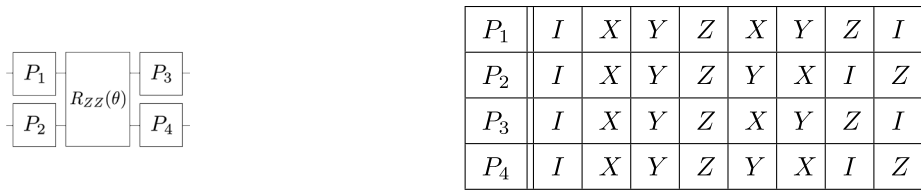
Extended Data Fig. 4 | MPS circuit simulations of scattering in one-dimensional Ising field theory. The vacuum-subtracted energy density E_n throughout the scattering process for a selection of center-of-mass energies E_{tot} . The initial wavepackets are separated by 10 sites and evolved with a Trotter time

step of $\delta t = 1/16$. The wavepackets are constructed from 8 steps of ADAPT-VQE except for $k_0 = 0.2\pi$ which is constructed from 10 steps. Results for $L = 256$ and $\sigma = 0.13$, $d = 22$, $g_x = 1.25$, $g_z = 0.15$ and max bond dimension 350 are shown.

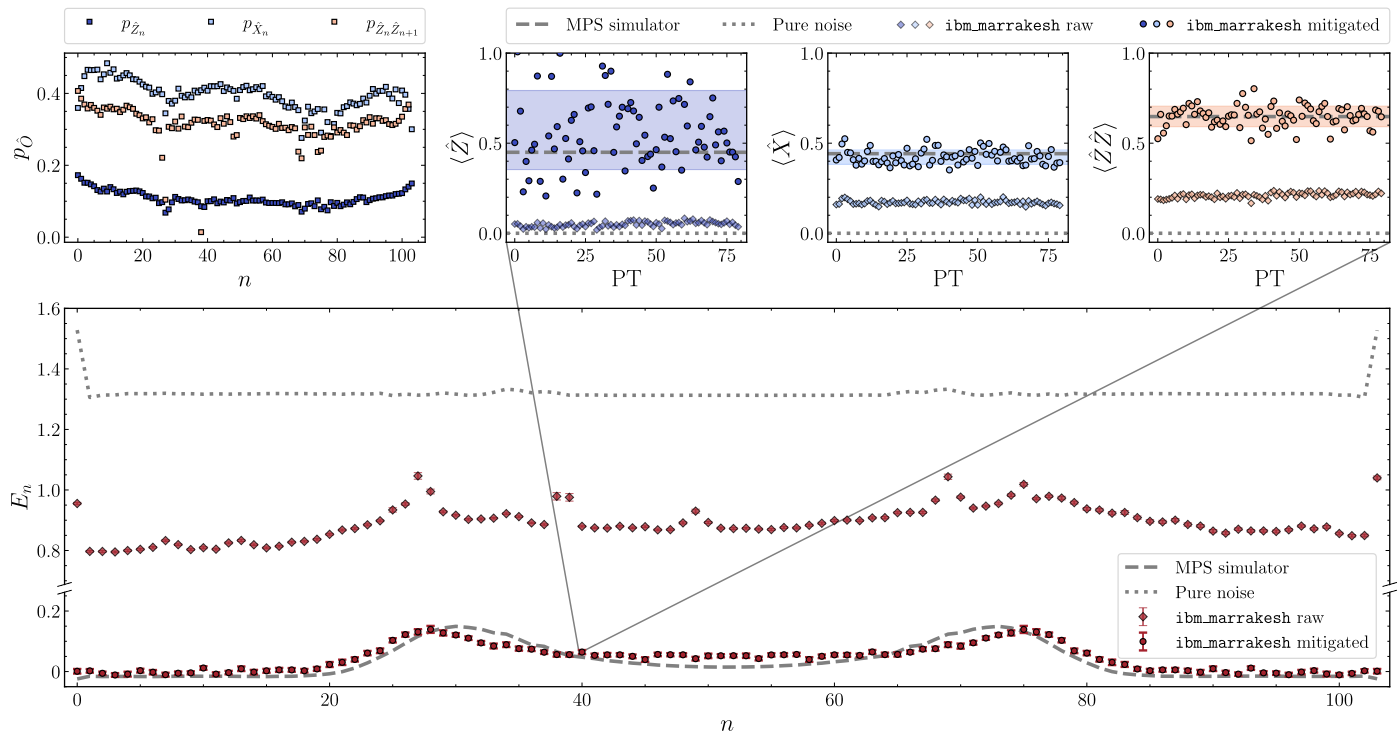


Extended Data Fig. 5 | Comparison of OBCs and PBCs in one-dimensional Ising field theory. Left: the vacuum-subtracted energy density E_n throughout a MPS simulation of scattering on a $L=100$ lattice with OBCs. Wavepacket

parameters $\sigma = 0.13$, $k_0 = 0.36\pi$ and a time step of $\delta t = 1/16$ are used. Right: the energy density at $t = 20$ and $t = 30$ for OBCs (blue) and periodic boundary conditions (PBCs) (tan).

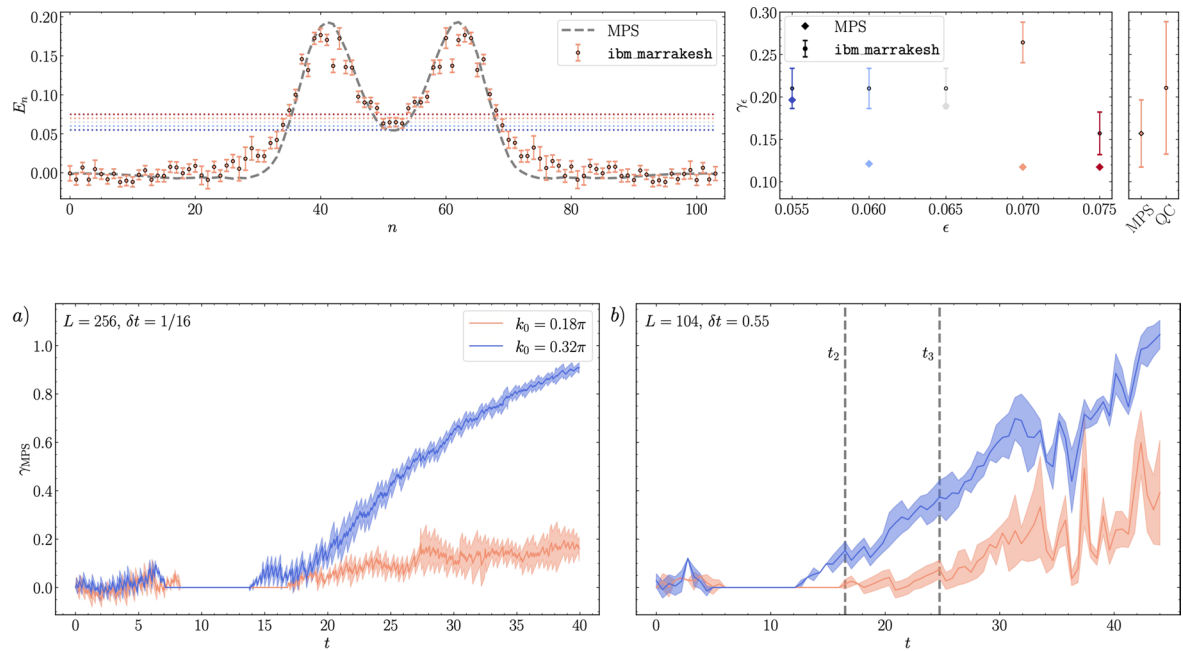


Extended Data Fig. 6 | Pauli twirling of the $R_{ZZ}(\theta)$ gate. The Pauli gates P_i are appended before and after $R_{ZZ}(\theta)$ as shown on the left. The table on the right shows the sets of P_i that leave $R_{ZZ}(\theta)$ invariant for all θ .



Extended Data Fig. 7 | The effect of error mitigation on the quantum simulation results from `ibm_marrakesh`. The data corresponds to the quantum simulation results in Fig. 4 for $L=104$ and $t_3=24.75$ (130 two-qubit gate depth). Top left: the median signal strengths p_O defined in Eq. 25 as a function of lattice position n for $O = Z_n, X_n, Z_n Z_{n+1}$. The signal strength is computed for each n by averaging over the TREX twirls, and then computing the median over the set of PTs. Top right: the effect of ODR on the expectation values of the same O for one lattice site, $n=40$. The data points are determined by averaging over TREX twirls

for each PT. The gray dotted lines represent the expectation value of a completely decohered state, while the gray dashed lines are the MPS predictions. The colored bands represent ± 1 standard deviation of the mitigated results. Bottom: the vacuum-subtracted energy density E_n of the raw device data (diamonds) and after all error mitigation (circles). The raw device data represents the median over PTs (averaged over TREX twirls). The error bars for both the raw and the mitigated data are obtained via bootstrap resampling.



Extended Data Fig. 8 | Calculation of skewness to indicate inelasticity. Upper: Calculation of skewness for $t_2 = 16.5$. Left: the range of energy cutoffs ϵ (dotted lines) are overlaid on the energy density from Fig. 4. The sample size is 1.28×10^6 and the statistical error bars are the bootstrap standard error centered around the mean. Middle: the third moment of the energy density distribution γ_ϵ is calculated for a contiguous interval of points where $E_n + \sigma_n \geq \epsilon$. The error bars represent the standard deviation computed via bootstrap resampling centered around the mean. Right: the reported value of γ is computed via Eq. 28, with error bars centered at the mean that cover the range of γ_ϵ coming from the variation

of the energy cutoff and, for the quantum results, statistical errors from the bootstrap standard error. Lower: Skewness as an indicator of inelasticity. **a)** The skewness γ_{MPS} calculated for MPS simulations of elastic ($k_0 = 0.18\pi$) and inelastic ($k_0 = 0.32\pi$) scattering with $L=256$, $\delta t=1/16$, $d=27$, $\sigma=0.1$, PBCs, and max bond dimension 350. The energy cutoffs ϵ are chosen to be $[E_{L/2} + 0.01, E_{L/2} + 0.03]$ in increments of 0.005, and γ_{MPS} is set to 0 if the maximum value of E_n occurs at $L/2$ or if there are no points with $E_n > \epsilon$. **b)** The same but for $L=104$, $\delta t=0.55$, $d=21$, $\sigma=0.13$, OBCs, and a max bond dimension 1,500. The vertical lines show the times $t_2 = 16.5$ and $t_3 = 24.75$ at which the skewness in Fig. 5 is calculated.