

Benchmarking digital quantum simulations and optimization above hundreds of qubits using quantum critical dynamics

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The real-time simulation of large many-body quantum systems is a formidable task, that may only be achievable with a genuine quantum computational platform. Currently, quantum hardware with a number of qubits sufficient to make classical emulation challenging is available. This condition is necessary for the pursuit of a so-called quantum advantage, but it also makes verifying the results very difficult. In this manuscript, we flip the perspective and utilize known theoretical results about many-body quantum critical dynamics to benchmark quantum hardware and various error mitigation techniques on up to 133 qubits. In particular, we benchmark against known universal scaling laws in the Hamiltonian simulation of a time-dependent transverse field Ising Hamiltonian. Incorporating only basic error mitigation and suppression methods, our study shows coherent control up to a two-qubit gate depth of 28, featuring a maximum of 1396 two-qubit gates, before noise becomes prevalent. These results are transferable to applications such as digitized quantum annealing and match the results of a 133-site optimization, where we identify an optimal working point in terms of both circuit depth and time step.

I. INTRODUCTION

Quantum critical dynamics occur when a quantum system reaches a critical point (CP), characterized by a non-analytic change in the system’s ground state energy as a function of a Hamiltonian parameter. The system’s correlation length and relaxation time are maximal at the CP and diverge in the thermodynamic limit. Crossing it, the system undergoes a quantum phase transition (QPT). As a result, system details no longer affect macroscopic quantities, causing the emergence of universal behavior, a key property of critical phenomena [1–3].

QPTs are experimentally realized by changing the control parameters of the system Hamiltonian over time. However, understanding the real-time dynamics of many-body quantum systems close to the critical point is a formidable task. Many believe that only quantum simulators [4], i.e., controllable quantum systems that can emulate others [5], can tackle this problem at scale [6, 7]. Quantum simulators were first realized with ultracold dilute gas in an optical lattice [8] and have since been implemented on a variety of platforms [6, 7, 9–11]. Most of these platforms are *analog* quantum simulators, which are subject to calibration errors and decoherence.

A parallel approach is to perform the simulation on *digital* quantum computers using suitable algorithms compiled to the native basis gate set of the hardware [12–17]. However, current digital machines are prone to errors, such as calibration errors, cross-talk, and decoherence. In the future, quantum error correction could potentially enable fault-tolerant simulations of many-body quantum

systems on digital machines [18]. Ref. 19 gives a perspective on the relative strengths and weaknesses of analog and digital platforms.

Crucially, quantum critical dynamics have implications beyond condensed matter and statistical physics. For example, QPTs occur ubiquitously in quantum optimization, where a quantum algorithm helps solve a classical optimization problem. Such applications are among the most anticipated and economically impactful use cases for quantum computers [20]. Quantum annealing (QA) is an algorithm to find ground states that can be used to solve combinatorial optimization problems [21]. It evolves an easy-to-prepare ground state of one Hamiltonian to the unknown ground state of another problem Hamiltonian, which corresponds to the classical optimization problem to solve. If the evolution is adiabatically slow, the system follows the instantaneous ground state of the time-dependent Hamiltonian and ends in the solution of the optimization problem. Particularly for QA, QPTs create algorithmic bottlenecks [21–23], as they imply an energy gap between the ground and the first excited state that closes in the thermodynamic limit. For finite annealing times t_f , the evolution may therefore not be adiabatic due to a diverging relaxation time at the CP. This mechanism produces defects that carry through to the final state [24].

The quantum Kibble-Zurek mechanism (QKZM) [24–26] quantifies the relationship between t_f and the number of defects produced during the annealing run. It predicts a universal scaling, a power-law decay, of the density of defects in the final solution as a function of t_f and the system’s critical exponents [27], i.e., a set of numbers characterizing the system’s behavior near its CP. It has been the subject of a range of largely analog experimental studies [28–31].

We first present an application-oriented benchmarking

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method that utilizes the predictability and universality of the Kibble-Zurek (KZ) scaling. Those attributes make it ideal for an intuitive and easily scalable metric to assess the quality of large-scale quantum simulations. This is increasingly important as digital quantum computing devices and algorithms have left the infantile stage of a few tens of qubits with error rates prohibiting more than a handful of two-qubit gates [32, 33]. Today’s quantum devices can exceed 100 qubits at error rates that, combined with error mitigation and suppression (EMS) techniques [34], allow a coherent simulation of thousands of two-qubit gates [14, 35].

Many benchmarking methods employ randomized circuits. This makes them more comparable, objective, and device-agnostic while accounting for, e.g., qubit connectivity and basis gate set [36]. Moreover, randomness helps collect many of the error sources into the same benchmarking process. Examples of such methods span an entire field of research, including variants of randomized benchmarking [37–39], cross-entropy benchmarking [40], and quantum volume [41]. These methods are crucial to assess gate fidelities and characterize different kinds of noise. However, they do not appropriately represent the capabilities of current quantum hardware to run a specific application. Indeed, applications for noisy quantum devices have circuits with highly structured repeated layers that are often tailored to the connectivity and the basis gate set of the hardware. It is therefore of little surprise that such simulations achieve much higher gate counts and qubit numbers than one would predict from generic benchmarks. Even though there are very promising new benchmarking methods designed to overcome these issues [42], they still only provide a fidelity without relating to applications. Pure application benchmarks are the other extreme. Either by testing against a set of well-understood problems and, possibly, corresponding solutions [43, 44], or based on specific applications such as quantum optimization [45] or discrete time crystals [46].

We go a step further and propose a concrete, application-oriented benchmarking scheme to assess how many two-qubit gate layers of a given application circuit can be coherently simulated given a specific device and, importantly, EMS method. A schematic of the principle is shown in Fig. 1a. The result is not an abstract fidelity but simply the number of circuit layers that can be reliably simulated, which can be directly transferred to other applications.

Next, we apply this benchmark to combinatorial optimization as an application of QA. Although hardware limitations have shifted attention towards the quantum approximate optimization algorithm (QAOA), QA remains an excellent candidate to achieve a computational advantage in quantum optimization [47, 48]. QAOA is an annealing-inspired variational ansatz, with variational layers representing time steps in digitized QA, used in conjunction with a variational quantum eigensolver (VQE) [49]. Recent studies indicate that solving hard op-

timization problems requires many QAOA layers [50, 51]. At the same time, the optimally converged parameter values of QAOA in the large-layer limit reproduce annealing schedules, meaning QAOA implements digitized QA with variationally found annealing schedules. It is therefore important to better understand digitized QA. An important question is whether the algorithmic error stemming from a finite time step can improve the efficiency, similar to what happens in simulated QA [47]. Here, we identify an optimal working point with respect to the time step and number of circuit layers to minimize the residual energy given the finite hardware resources and how it depends on the system’s minimum energy gap.

In summary, we explore two directions – benchmarking and optimization. Section II provides the necessary technical background to QA, the QKZM, and Trotterized time evolution. In Section III, we introduce and implement our application-oriented benchmark of quantum simulation against universal behavior. Here, we present the main results of this work – a comparison of different levels of EMS on two quantum processors with up to 133 qubits using our QKZM-based benchmarking. Section IV studies digitized QA for solving optimization problems and the effect that the time step has on the quality of the solution. We identify optimal time steps in the presence of different minimum energy gaps on 12 qubits in Section IV A and on systems with up to 133 qubits in Section IV B. We conclude in Section V.

II. DIGITIZED QUANTUM ANNEALING AND DEFECT PRODUCTION

Given a (mixing) Hamiltonian H_M with an easy-to-prepare ground state and a problem Hamiltonian H_P whose ground state we wish to compute, we construct a time-dependent combination of the two,

$$H(s) = A(s)H_M + B(s)H_P . \quad (1)$$

Here, $s = t/t_f$ is the time $t \in [0, t_f]$ rescaled by the total annealing time t_f . $A(s)$ and $B(s)$ are the annealing schedules such that $H(0) = H_M$ and $H(1) = H_P$. The system is initially prepared in the ground state of H_M and evolved for time t_f . If this evolution is adiabatically slow, i.e., for large enough t_f , the system remains in the ground state of the instantaneous Hamiltonian and ends in the desired ground state of H_P at $t = t_f$ [21].

The prototypical Hamiltonian considered in QA is an N -site transverse field Ising model (TFIM) with nearest-neighbor interactions,

$$H_M = - \sum_i \sigma_i^x , \quad H_P = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z , \quad (2)$$

with Pauli matrices σ_i^x and σ_i^z acting on site i and couplings J_{ij} between nearest neighboring sites indicated by $\langle i, j \rangle$. The ground state of $H(0) = H_M$ is $|+\rangle^N$. We apply linear schedules $A(s) = (1 - s)$ and $B(s) = s$ for simplicity,

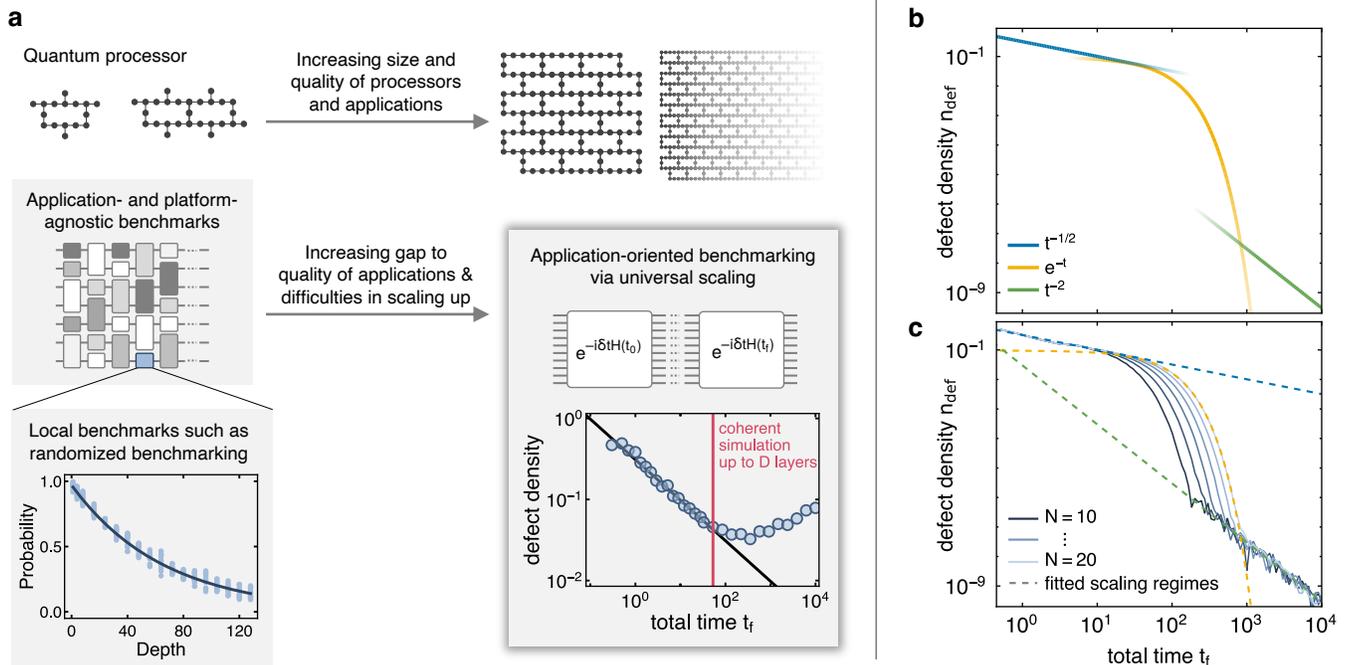


FIG. 1. **Application-oriented benchmarking of quantum simulations.** **a** Benchmarking experiments give detailed insight into device characteristics such as error rates and decoherence times. As devices scale, however, it is desirable to have a benchmarking method that resembles the applications that are executed. By simulating critical dynamics and measuring an observable that follows a known universal scaling, we track for how many time steps, which correspond directly to the number of circuit layers, we can reproduce the expected universal scaling. Here, we measure the density of defects produced in quantum annealing, predicted by the Kibble-Zurek scaling. This provides a direct and concrete metric predicting how many layers of two-qubit gates can be coherently simulated given, e.g., a certain device, qubit subset, and error mitigation technique. **b** For finite system sizes away from the thermodynamic limit, the density of defects exhibits two scaling regimes beyond the Kibble-Zurek scaling that are theoretically known (see main text). These can benchmark deep circuits. **c** The departure from Kibble-Zurek scaling is determined by the system size and all three scaling regimes can be identified in statevector simulations with $N = 10, \dots, 20$ spins (solid lines).

resulting in

$$H(s) = -A(s) \sum_i \sigma_i^x - B(s) \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z. \quad (3)$$

Unless otherwise stated, we consider an ordered Ising model with uniform couplings $J_{ij} \equiv J$.

The TFIM is the simplest model exhibiting a QPT [2] in the thermodynamic limit $N \rightarrow \infty$. In the simple case of uniform couplings $J > 0$ ($J < 0$), the CP at $J_c = A/B$ separates the paramagnetic phase ($A \gg JB$) from the doubly-degenerate (anti-)ferromagnetic phase ($A \ll JB$) with all spins (anti-)aligned. In the disordered case, the latter is substituted by a glassy phase, i.e., an energy landscape with many deep local minima [23].

A. The Kibble-Zurek mechanism

The QKZM describes the non-equilibrium dynamics of the systems in the realistic setting of crossing this CP with finite annealing time t_f , leading to defects in the final solution. Ref. 24 provides an excellent account of the

QKZM and the resulting density of defects scaling in a TFIM, both by employing the original (classical) reasoning of the Kibble-Zurek mechanism (KZM) and in terms of a fully quantum description based on Landau-Zener (LZ) theory. Here, a defect refers to the wrong orientation of a spin and the density of defects to the number of defects averaged over all sites. We now summarize the classical description of the KZM following Ref. 24. Classically, the CP is characterized by a diverging correlation length ξ and relaxation time τ . Far away from the CP, τ is small enough for the system to instantaneously relax to equilibrium. As the system approaches the CP, τ becomes equal to and, eventually, grows beyond the time scale on which H changes. When this happens, the system can no longer relax to its instantaneous ground state, with reactions to changes slowing down until they halt completely. This is usually referred to as the critical slowdown and subsequent freezing out. Past the CP, as τ decreases again, the system unfreezes and, crucially, continues evolving from approximately the frozen-out state, resulting in defects in the final state. In summary, the growth of the system's relaxation time at

the CP, which is finite for finite system sizes, determines the necessary rate of change of the system $ds/dt = 1/t_f$ required to track the instantaneous ground state. This is the essence of the KZM. It predicts the density of defects as a function of a finite annealing time t_f with a power-law decay [27, 29]

$$n_{\text{def}} \propto t_f^{-\frac{d\nu}{1+z\nu}}, \quad (4)$$

fully determined by the system dimension d and its critical exponents ν and z . In 1D, with $d = 1, z = 1, \nu = 1$, this becomes

$$n_{\text{def}} \propto t_f^{-1/2}. \quad (5)$$

In the quantum description, the existence of a QPT and all its related quantities originate from the closing of the system's energy gap at the CP. For finite system sizes $N < \infty$, the minimum gap between the ground state and the first excited state is small but finite and decreases as $\propto 1/N$. It closes in the thermodynamic limit $N \rightarrow \infty$, causing both the correlation length ξ and relaxation time τ to diverge. Assuming annealing times fast enough to produce at least one defect on average, LZ theory yields the same KZ scaling in a quantum setting [24].

For uniform couplings J , defects in the ferromagnetic solution after annealing appear as pairs of spins with opposite sign and can be measured by $\sigma_i^z \sigma_j^z$ correlators over all N_e edges of the spin-lattice, i.e., all nearest-neighbor correlators,

$$n_{\text{def}} = \frac{1}{2N_e} \sum_{\langle i,j \rangle}^{N_e} (1 - \sigma_i^z \sigma_j^z). \quad (6)$$

For example, an open chain of N spins has $N_e = N - 1$ edges and a periodic chain has $N_e = N$ edges.

B. Density of defect-scaling across various regimes

For finite system sizes and slow anneals, i.e., large t_f , Ref. 24 describes an exponential drop in defect density following the regime of KZ scaling that is captured by LZ dynamics. In that case, when the anneal is slow enough to never freeze out and to produce less than one defect in the chain on average, the number of defects is proportional to the LZ probability p_{LZ} of exciting the system,

$$n_{\text{def}} \propto p_{\text{LZ}} \approx \exp\left(-b \frac{t_f}{N^2}\right), \quad (7)$$

with b a constant. Following Refs. 52, 53, for adiabatically slow anneals, i.e., even larger t_f , the scaling reads

$$n_{\text{def}} \approx p_{\text{LZ}}(t_f) + \frac{1 - 2p_{\text{LZ}}(t_f)}{at_f^2}, \quad (8)$$

where a is a constant. The expressions of constants a and b can be found in Refs. 24, 53.

The theoretical predictions for the three scaling regimes in Eqs. (5), (7) and (8) are shown in Fig. 1b. Density of defects scalings obtained from ideal statevector simulations in Fig. 1c with system sizes up to $N = 20$ spins show that the beyond-KZM scaling regimes, i.e., Eqs. (7) and (8) are finite-size effects and that their onset is controlled by the system size.

C. Product formulas for time-dependent Hamiltonians

Ultimately, QA implements the time evolution under a time-dependent Hamiltonian $H(t)$. The unitary time evolution operator obtained by integrating the time-dependent Schrödinger equation reads

$$U(t_f, t_0) = \mathcal{T} \exp\left(-i \int_{t_0}^{t_f} dt' H(t')\right). \quad (9)$$

The time-ordering \mathcal{T} accounts for any non-commutativity of the Hamiltonian with itself at different times, $[H(t), H(t')] \neq 0$.

To implement QA on a digital quantum computer, we must decompose Eq. (9) into quantum gates [12]. The simplest digitized implementation of Eq. (9) for a Hamiltonian $H(t) = \sum_{l=1}^L a_l(t) H_l$ is via a first order product formula (PF), which approximates the integral as a Riemann sum, $\int_0^{t_f} dt' H(t') = \lim_{n \rightarrow \infty} \sum_{m=1}^n H(m\Delta t) \Delta t$ with $\Delta t = t_f/n$ [54, 55]. Importantly, the time ordering in the Trotterized $U(t_f, t_0)$ is enforced with a “right-to-left ordering”, resulting in

$$U \approx \prod_{m=n}^1 e^{-i\Delta t \sum_l a_l(m\Delta t) H_l}. \quad (10)$$

Therefore, in contrast to the case of a time-independent Hamiltonian, splitting the exponent into discrete time steps introduces a first approximation. Typically, a digital quantum computer cannot natively implement e^{-itH} . Therefore, the Hamiltonian at time step $m\Delta t$ is further decomposed using a first order PF, or any higher-order PF,

$$U \approx \prod_{m=n}^1 \prod_{l=1}^L e^{-ia_l(m\Delta t) H_l \Delta t}. \quad (11)$$

Each of these exponentials can be directly represented by the hardware native basis gates of the digital machine. Note that, in principle, any other quantum algorithm for quantum dynamics could be used to decompose the time evolution operator as long as it allows for time-dependent Hamiltonians [12, 56].

III. APPLICATION-ORIENTED BENCHMARKING THROUGH UNIVERSAL SCALING

Here, we suggest a direct approach to benchmark close to applications. We simulate the time evolution under a time-dependent Hamiltonian and benchmark the accuracy with which a known universal scaling is replicated. A schematic of our method is shown in Fig. 1a. We propose to measure the density of defects after digitized QA as a function of total annealing time t_f . Given a fixed time step, the time t_f directly corresponds to the number of circuit layers in the Trotterized time evolution circuit. The density of defects will decrease according to the predicted scaling up to a certain threshold t_f , after which hardware noise dominates. This causes decoherence of the system and an increase of n_{def} , deviating from the predicted KZ scaling. Many other theoretical and experimental studies of the effect of dissipation on the KZ scaling confirm this increase [27, 30, 57]. The number of circuit layers for which the expected scaling of n_{def} is observed is the number of circuit layers for which coherent simulation was achieved.

This benchmark has several advantages. First and foremost, it yields a concrete, intuitive, and scalable metric; the number of simulable circuit layers as they can be found in countless applications. Even more so since Hamiltonian simulation is a prime application for quantum computers and a building block for many other applications, for example, quantum phase estimation [58] and sampling algorithms [59]. Second, our method can benchmark hardware and EMS algorithms separately or in combination. Third, our method is scalable since no classical verification is required. Fourth, since the KZ scaling is defined in the thermodynamic limit $N \rightarrow \infty$, it is particularly well-suited to benchmark large digital quantum computers without scaling issues. Finally, since finite-size scaling regimes are also well-understood (cf. Section II B and Fig. 1b,c), the method is applicable in the setting of scaling to large circuit depths at qubit counts far below the thermodynamic limit.

A. Experimental setup

We now discuss benchmarking different levels of EMS on two quantum processors through digitized QA and measuring defect densities. An N -spin Ising model with uniform couplings $J = 1$ and linear schedules (cf. Section II) is mapped to N qubits. The qubit register is initialized as $\psi(t = 0) = |+\rangle^N$, the ground state of $H(t = 0) = H_M$, and time evolved under the time-dependent Hamiltonian in Eq. (3). The time evolution is implemented using a first-order PF as in Eq. (11) with a time step of Δt . Throughout this section, we use a time step of $\Delta t = 0.5$, which in our experience is sufficiently small to avoid significant algorithmic errors while, at the same time, allowing for larger annealing times.

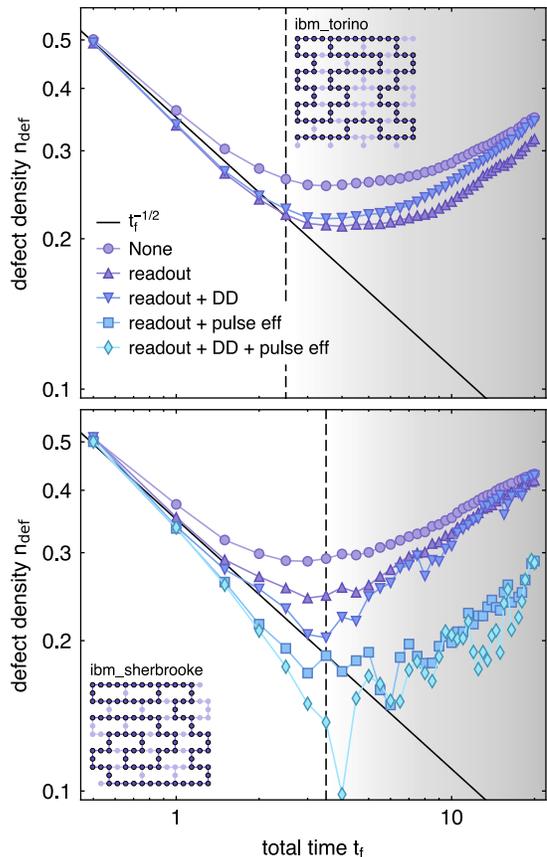


FIG. 2. **Density of defects scaling in 1D from 100-qubit circuits.** Hardware results comparing the density of defects scaling on subsets of 100 qubits on `ibm_torino` (top) and `ibm_sherbrooke` (bottom) employing different levels of EMS. Each point corresponds to one additional Trotter layer or time step of $\Delta t = 0.5$. Raw simulation results with no EMS (None) are compared to results using combinations of REM, DD error suppression, and pulse-efficient transpilation. Insets show the qubit layout of the respective processor with the chosen qubit subset highlighted. The black dashed line indicates the threshold time t_f until which the simulation stayed true to the expected KZ scaling, shown by the black solid line.

After annealing for a total time t_f , we measure the defect density via Eq. (6) to compare to the expected scaling in Eq. (5). Expectation values of observables are estimated from measurements with QISKIT's Estimator primitive [60].

We employ the IBM Heron processor `ibm_torino` and the IBM Eagle processor `ibm_sherbrooke` for our simulations, with 133 and 127 qubits, respectively, and heavy-hexagonal qubit connectivity [61]. Hardware characteristics such as error rates are given in Appendix B. Eagle and Heron processors differ in their native two-qubit gates and how they are physically realized. `ibm_sherbrooke`'s native two-qubit gate is an echoed cross resonance (ECR) gate implemented via a dispersive coupling mediated by a fixed-frequency resonator [62, 63]. By contrast, `ibm_torino`'s native two-qubit gate is a CZ

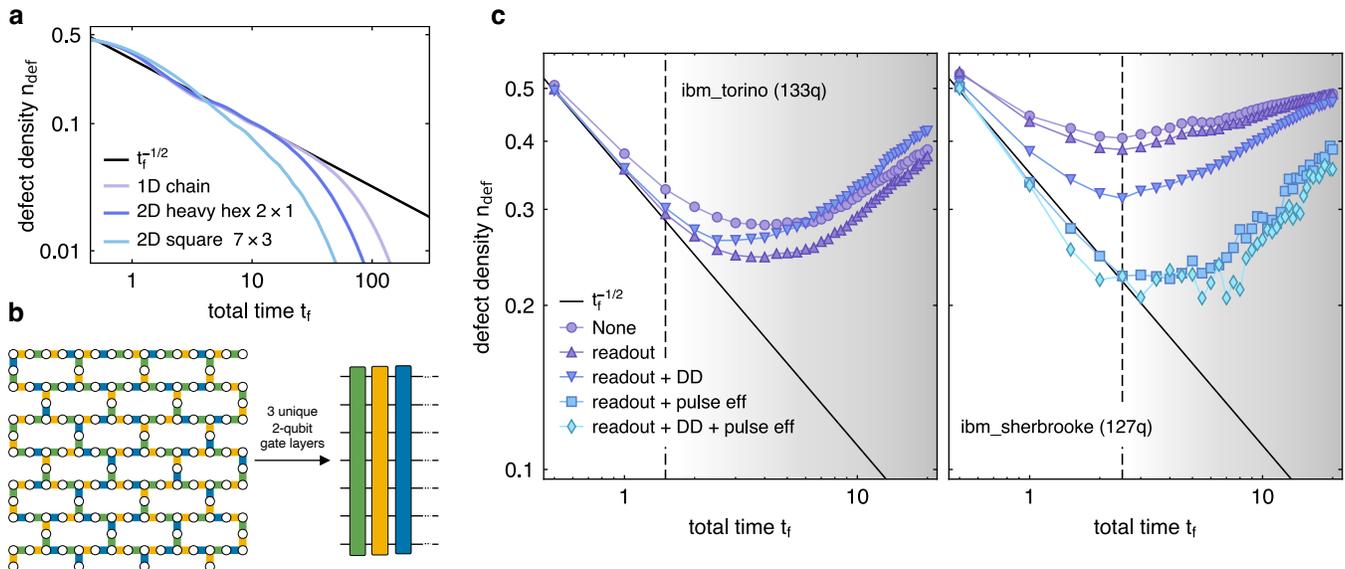


FIG. 3. **Density of defects scaling on a heavy-hexagonal lattice from 133- and 127-qubit circuits.** **a** Statevector results comparing the density of defects scaling in a periodic chain, a heavy-hexagonal lattice consisting of two heavy-hex cells (2×1), and a 7×3 square lattice, all with $N = 21$ spins. The heavy-hexagonal lattice exhibits the same $t^{-1/2}$ scaling as predicted for 1D systems, whereas defects in a true 2D lattice show a steeper scaling. **b** The couplings on the heavy-hexagonal lattice of `ibm_torino` and `ibm_sherbrooke` are grouped such that each Trotter layer consists of three layers of R_{ZZ} gates. **c** Hardware results comparing the density of defects scaling on `ibm_torino` (left) and `ibm_sherbrooke` (right) employing different levels of EMS. Each point corresponds to one additional Trotter layer or time step of $\Delta t = 0.5$. Raw simulation results with no EMS (None) are compared to results using combinations of REM, DD error suppression, and pulse-efficient transpilation. The black dashed line indicates the time t_f until which the simulation stayed true to the expected KZ scaling, shown by the black solid line.

gate realized through tunable-frequency couplers. In a tunable coupler architecture, the coupling element is frequency tunable, and driving it can create different two-qubit gates [64, 65]. Most importantly, this results in `ibm_torino` having a roughly $6\times$ shorter two-qubit gate time compared to `ibm_sherbrooke` and a higher two-qubit gate quality [42].

On both devices, we compare simulations with no EMS to readout error mitigation (REM) [66, 67] as well as to REM combined with dynamical decoupling (DD) [68]. In addition, `ibm_sherbrooke` allows for pulse-efficient transpilation of our circuits, another method of error suppression [69]. Pulse-efficient transpilation scales hardware native cross-resonance pulses and their echoes (combined, this makes up an ECR gate on `ibm_sherbrooke`) and is thus not compatible with `ibm_torino`'s native CZ gates. Appendix A gives a brief technical summary of each method.

B. Results: 1D chain

The Trotter circuit for the time evolution of a spin chain requires at least two layers of R_{ZZ} gates per Trotter layer, or time step. Since each R_{ZZ} gate is transpiled to two hardware native two-qubit gates (ECR or CZ), the final circuit for a 1D Ising model has a two-qubit gate

depth of $4 \times N_t$ where N_t is the number of time steps. Fig. 2 shows the density of defects scaling obtained from digitized QA on subsets of 100 qubits connected through an open line (see insets), which was chosen to minimize cumulative two-qubit gate errors along the line (cf. Appendix B). Owing to noise, the experimental results differ from the noiseless statevector results in Fig. 1c, which show a monotonic decrease in defect density with increasing t_f . Hardware errors only make it possible to follow the KZ scaling and subsequent scaling regimes up to a certain threshold time indicated by the dashed horizontal line in Fig. 2. Beyond this point, the defect density rises again, as the noise accumulates with increasing circuit depth and the system decoheres (indicated by grey shading). This phenomenon has been observed in analog simulators based on superconducting qubits [27, 30], and predicted by continuous-time numerical simulations that incorporate dissipation [57]. Nevertheless, this is the first time that the existence of such an optimal working point has been observed in digital quantum simulations.

This threshold time depends on the hardware and the EMS employed. The top panel of Fig. 2 shows the results for `ibm_torino` comparing no EMS with only REM, and with REM combined with DD. While we can simulate two Trotter layers with a two-qubit gate depth of 8 and a total of 396 CZ gates without any level of EMS, adding REM already significantly improves the results.

We can reliably simulate up to five Trotter layers with a two-qubit gate depth of 20 and 990 CZ gates in total. Assuming `ibm_torino`'s median CZ gate time of 84 ns for all two-qubit gates, this implies a coherent simulation of 1.7 μ s. This is remarkable given that REM is the simplest and easiest-to-implement form of error mitigation (EM). We attribute the negligible impact of the DD sequence on the `ibm_torino` results to the reduced cross-talk of the device compared to `ibm_sherbrooke`.

The picture is different on `ibm_sherbrooke`, shown in the bottom panel of Fig. 2. We compare the same EMS methods as on `ibm_torino` in addition to pulse-efficiently transpiled circuits. The results without any EMS and only REM are slightly worse than on `ibm_torino`. However, adding DD to counter static ZZ cross-talk results in substantial gains on this device. We achieve a coherent simulation of seven circuit layers with a two-qubit gate depth of 28 and 1386 ECR gates in total. Assuming `ibm_sherbrooke`'s median ECR gate time of 533 ns [61] for all two-qubit gates, this equates to a coherent circuit execution time of roughly 15 μ s. Moreover, we show in Appendix D that the correlations between defects show the characteristic non-monotonic fingerprint of a genuine quantum KZM. Pulse-efficient transpilation fairs similarly, though we observe that the curve dips below the expected scaling. We attribute this to rotation errors in the scaled two-qubit pulses at small angles [69], see Appendix A. As the two-qubit gate angles $\theta = -2JB(m\Delta t/t_f)\Delta t = -2Jm\Delta t^2/t_f$, with $m\Delta t = t$, are proportional to the annealing schedule, increasing t_f means smaller and smaller angles at the beginning of an anneal. This causes a growing disparity between the target operation of the circuit before transpilation and the final sequence of gates with growing t_f . Fixing these rotation errors requires custom calibrations [70], which are difficult at scale through a cloud-based quantum computing service. Since our goal is to compare out-of-the-box EMS methods, we did not conduct any custom calibrations.

C. Results: heavy-hexagonal lattice

Our approach is not limited to one-dimensional spin systems. In fact, such critical behavior and the resulting universal scaling manifests in lattice geometries beyond 1D [71] and can hence benchmark any qubit connectivity for which the critical exponents and scaling are known. The processors we use have a heavy-hexagonal qubit connectivity for which we need to infer the predicted KZ scaling. The degree of connectivity, i.e., the number of edges over the number of sites, in a heavy-hex graph is $N_e/N_s = 6/5 = 1.2$. In terms of connectivity, it is hence much closer to a 1D system with $N_e/N_s = 1$ than to a 2D square lattice with $N_e/N_s = 2$. We therefore conclude that the density of defects on a heavy-hex lattice should follow a scaling similar to the 1D scaling of $t^{-1/2}$. This is further supported by noiseless statevector simu-

lations shown in Fig. 3a comparing the density of defects scaling of a 1D periodic chain, a heavy-hex lattice, and a 2D square lattice with $N = 21$ sites each. The data shows that the density of defects in 1D and heavy-hex lattices coincide on the $t^{-1/2}$ scaling before the exponential drop-off at larger t_f , attributed to finite-size effects, while the 2D square lattice shows a steeper scaling. This is why we reasonably consider the $t^{-1/2}$ scaling also as the benchmark line for the heavy-hex lattice, even though deviations from the exact $t^{-1/2}$ scaling are possible for this geometry and the critical exponents should be further investigated.

The Trotter circuit for a Hamiltonian Eq. (3) on a heavy-hex lattice is made depth-optimal by grouping the couplings according to the edge-coloring shown in Fig. 3b. Each Trotter layer in the circuit therefore consists of three layers of R_{ZZ} gates. Again, each R_{ZZ} gate is transpiled into two hardware-native two-qubit gates, resulting in a total two-qubit gate depth of $6 \times N_t$.

Utilizing all 133 and 127 qubits of `ibm_torino` and `ibm_sherbrooke`, respectively, we see an even starker difference between both chips in defect density (Fig. 3c). We can coherently simulate up to three Trotter layers on `ibm_torino` employing only REM. With 150 edges, this equals a two-qubit gate depth of 18 and 900 CZ gates in total. Again, assuming `ibm_torino`'s median CZ gate time of 84 ns for all two-qubit gates, this implies a coherent simulation of 1.5 μ s using merely REM. `ibm_sherbrooke`, on the other hand, requires more involved EMS, which becomes even more apparent when using all qubits of the device. Although DD again provides sizable improvements, we do not reproduce the expected KZ scaling. However, pulse-efficient transpilation combined with REM achieves five coherent Trotter layers. This is equivalent to a Trotter circuit with a CNOT gate depth of 30 and 1440 CNOT gates in total. In this case, the circuit duration reduces to roughly 6 μ s due to the pulse-efficient transpilation.

IV. DIGITIZED QUANTUM ANNEALING FOR OPTIMIZATION

The hardware and algorithms benchmarked in Section III C using a homogeneous ferromagnetic model have applications in combinatorial optimization. In this scenario, the couplings J_{ij} in Eq. (2) can be arbitrary in magnitude and sign. An optimization problem defined on this type of Hamiltonians may fall within the NP-complete complexity class, depending on the connectivity of the underlying graph, and are frequently employed as benchmarks for quantum optimization [48, 72]. It is therefore of interest to determine whether the results obtained from benchmarking the QKZM and identifying an optimal working point are transferable to an optimization context.

QA has been little explored on digital quantum computers. Instead, the focus has been mostly on QAOA, an

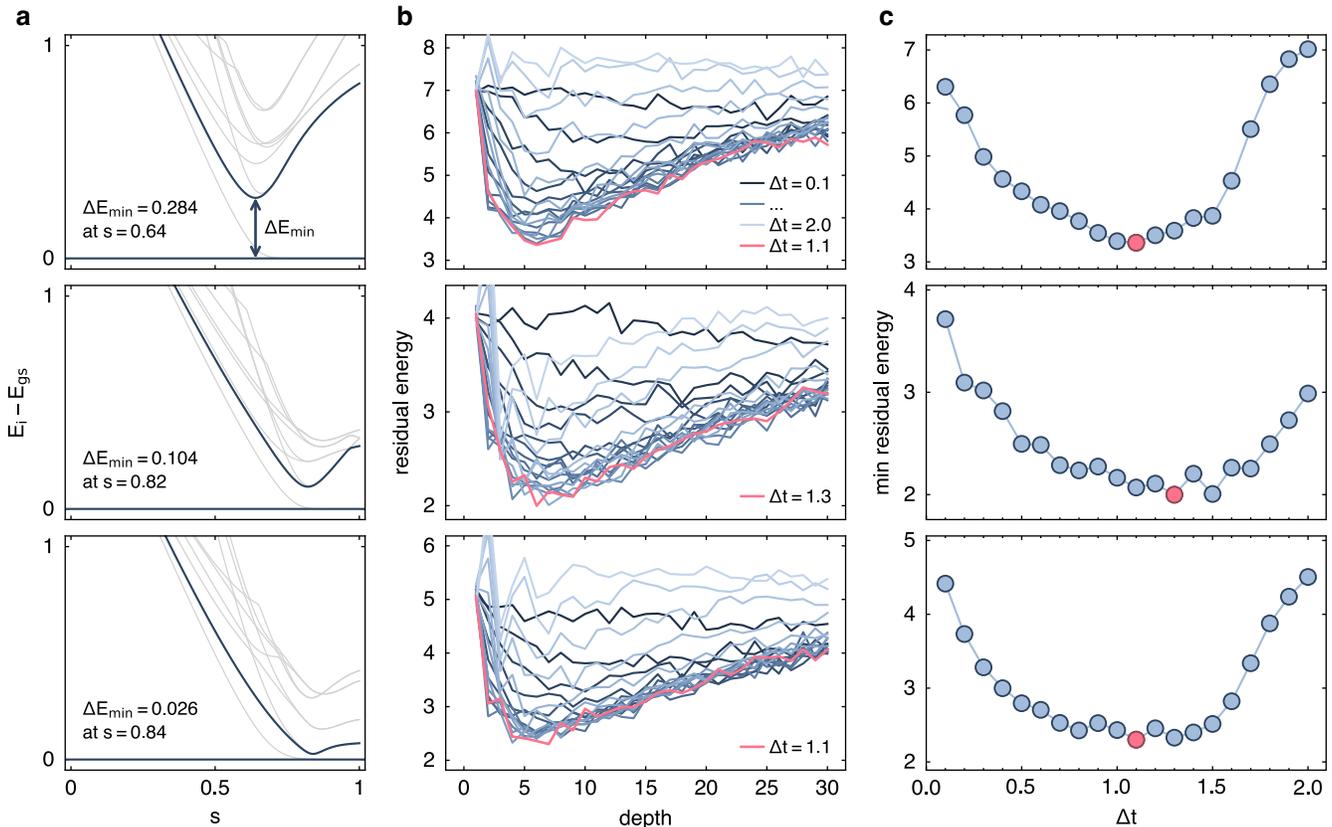


FIG. 4. **Hardware results of the residual energy dependence on time step and spectral gap.** **a** Spectra relative to the ground state of three different instances of disorder in a 12-qubit periodic chain with coupling coefficients uniformly sampled from $J_{ij} \in [-1, 1]$. The instances were specifically chosen with three different minimum energy gaps, differing by an order of magnitude between the largest (top) and the smallest gap (bottom). **b** Residual energy averaged over 400 samples obtained from QA of the system in **a** on `ibm_auckland` using only REM with fixed time steps $\Delta t \in \{0.1, \dots, 2.0\}$ as a function of circuit depth (number of time steps). **c** Minimum residual energy from **b** as a function of the time step, i.e., each point corresponds to the minimum over one curve in **b**.

annealing-inspired variational ansatz and the most popular near-term algorithm for quantum optimization [49, 68, 73, 74]. However, optimizing the variational parameters in QAOA is costly in itself [75] and, once found, optimal variational parameters reduce QAOA to QA in the large-layer limit [50]. This does not mean that the optimal QAOA parameters can be directly derived from annealing schedules. Rather, the variational optimization results in optimized annealing schedules. Nonetheless, precisely because of this relationship, annealing schedules can be used to initialize QAOA parameters, thereby reducing the training cost of the variational ansatz [75, 76]. It is therefore sensible to study digitized QA in more detail. Previous experimental realizations of digitized QA featured only up to nine qubits [77]. Since digitized QA requires discretizing the time evolution, the most central question is what effect does the choice of the time step have on the success of annealing?

The focus of this section is first to understand whether large algorithmic errors, i.e. large time steps, improve the performance of digitized QA. This effect has been observed in classical path-integral simulations of QA,

where an unconverged, finite Trotter step is beneficial for tunneling between configurations [47], reconciling earlier expectations of quantum speed-up [78] with observations [72]. Second, we identify an optimal time step for digitized QA given a fixed number of circuit layers or time steps N_t . Fixing N_t is meaningful, since, in reality, one has access only to a limited amount of resources such as the expendable number of gates, determining both the computational cost and, more importantly before achieving fault-tolerance, the amount of error introduced by hardware noise. At the same time, the success of QA relies on as large as possible annealing times t_f , which is achieved by increasing the time step Δt for a fixed number of time steps N_t . On the other hand, the errors of time evolution algorithms typically scale with Δt [12]. PFs are derived on the assumption of small time steps $\Delta t \ll 1$ and algorithmic errors scale with $\mathcal{O}(\Delta t^2)$ [55]. This naturally introduces a trade-off between QA performance and the algorithmic error due to Δt [76].

Since the solution to a classical optimization problem is a single bitstring, we are usually interested in individual measurement samples rather than expectation val-

ues. Therefore, we use QISKIT’s Sampler primitive [60] throughout this section to obtain individual measurement samples, i.e., bitstrings of measurement outcomes. Since many EM techniques apply only to expectation values, we only use REM in this section. Furthermore, we will compute the residual energy,

$$E_{\text{res}} = E(t_f) - E_0, \quad (12)$$

where $E(t_f) = \langle \psi(t_f) | H(t_f) | \psi(t_f) \rangle$ and E_0 is the exact ground state obtained through exact diagonalization for small system sizes and using CPLEX [79] for large systems.

A. Dependence of the residual on the time step and spectral gap

We first study the dependence of the digitized QA result on the time step on a small system of a periodic 12-qubit chain. Three instances of disorder with couplings randomly sampled from $J_{ij} \in [-1, 1]$ are chosen with varying minimum energy gaps between the ground and the first parity-preserving excited state since a smaller gap entails longer annealing times and makes finding a solution generally more difficult. Note that the Hamiltonian Eq. (3) and therefore its spectrum is a function of s . The minimum energy gap takes on its smallest value at the critical point. Furthermore, the first excited state of opposite parity becomes degenerate with the ground state as $s \rightarrow 1$. The spectra of the three different Hamiltonians as a function of s are shown in Fig. 4a with minimum gaps ranging across one order of magnitude. Fig. 4b displays the residual energy after annealing the respective system from a on `ibm_auckland` [80] with fixed time step $\Delta t \in \{0.1, \dots, 2.0\}$ as a function of the number of time steps (depth). Here, we observe that the smallest residual energies are reached after approximately 5 – 10 Trotter layers, owing to decoherence. For each Δt , the minimum residual energy achieved over all circuit depths is plotted in Fig. 4c. For all three systems, the lowest residual energy is obtained with a time step of $\Delta t > 1$, specifically $1.0 < \Delta t < 1.5$. Noiseless statevector simulations confirm that this is not merely a consequence of hardware noise, as seen in Appendix C, yielding an optimal time step of $1.2 < \Delta t < 1.4$. However, in statevector simulation, the existence of a finite optimal time step is likely due to the finite range of depths chosen. Therefore, choosing an infinitesimal time step seems to be both (i) inefficient in noise-free simulations and (ii) impractical in real experiments. On the other hand, a too-large time step implies algorithmic errors.

To summarize, we observe a trade-off between realizing the largest possible annealing times while keeping the algorithmic error under control. Choosing an unconverged, large time step is indeed advantageous when using digitized QA for optimization. This is of further relevance in the context of initializing QAOA variational parameters mentioned previously. In the context of directly studying

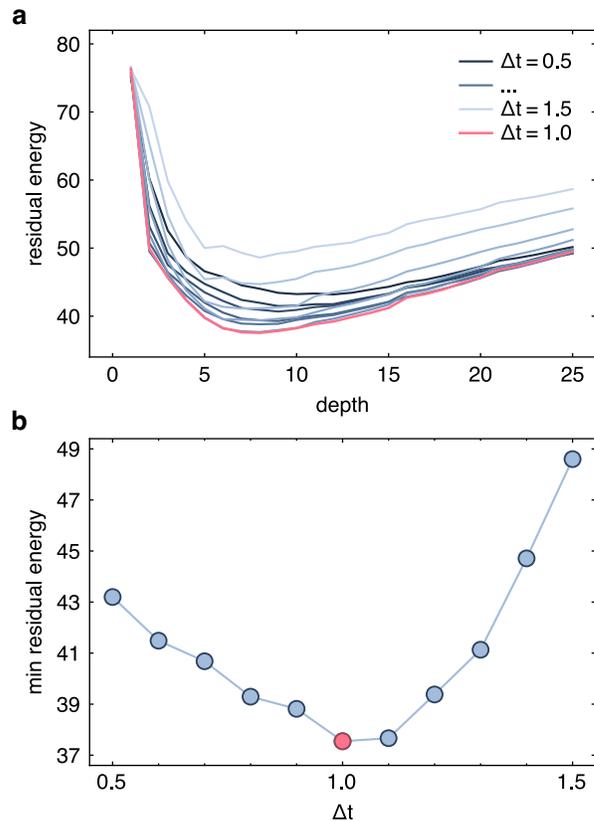


FIG. 5. **Hardware results of the residual energy dependence on the time step.** **a** Residual energy averaged over 10^5 samples obtained from QA on `ibm_torino` with fixed time steps $\Delta t \in \{0.5, \dots, 1.5\}$ as a function of circuit depth (number of time steps). **b** Minimum residual energy from **a** as a function of the time step, i.e., each point corresponds to the minimum over one curve in **a**.

QAOA performance, Ref. [76] finds an optimal time step of 0.75 for initializing variational parameters. Increasing Δt even further, however, does not provide any benefits as shown by the statevector results. This observation is consequential for practical noisy settings and allows us to optimize the number of Trotter steps needed to reach a target annealing time.

B. Optimization of disordered heavy-hexagonal graph

We now study a heavy-hexagonal spin-lattice of 133 qubits, i.e. `ibm_torino`’s full chip. We consider just one realization of disorder with uniformly sampled couplings $J_{ij} \in [-1, 1]$, and compute E_{res} as a function of circuit depth and time step as before. The ground state is again computed using CPLEX. This time, the system is too large to compute its instantaneous higher excited states, which is why we have no information about the size of its minimum energy gap. However, the comparison of different systems in the previous section indicates that

the dependence of the optimal time step on the spectral gap is small. Fig. 5a shows the results for time steps $\Delta t \in \{0.5, \dots, 1.5\}$. Again, we observe that, for each time step, the minimum residual energy is obtained at around 5 – 10 Trotter layers, or time steps, after which decoherence begins to dominate. This observation is compatible with both numerical predictions [57] and experimental results from analog simulation [30]. Furthermore, it is analogous to what was observed in the benchmarking experiment Fig. 3c. Fig. 5b reports the minimum E_{res} for each value of the time step. Also here, we observe a continuous decrease in E_{res} with increasing Δt up to a time step of 1.0 to 1.1, after which E_{res} sharply increases. In conclusion, this indicates an unconverged, large time step of $\Delta t \gtrsim 1.0$ to be optimal for digital QA regardless of the system instance and graph connectivity.

V. DISCUSSION AND OUTLOOK

This work presents an application-oriented method to jointly benchmark the hardware and the algorithms. Developing such a method to predict simulation quality, and, importantly, more closely resemble device and algorithm capabilities, is critical. Particularly so in times of rapid algorithmic and hardware advancements. The simple figure of merit that we introduce is the number of Trotter steps, i.e., the threshold depth, before which errors induce deviations from a universal scaling law. While we propose to use digitized QA and the universal KZ scaling in our work, we emphasize the central idea: benchmark against the prediction of a known universal behavior. Other scaling laws, model Hamiltonians, or lattice geometries could be employed as well.

We observe that different machines, equipped with different EMS, provide different threshold depths. Importantly, the simple benchmark we propose can measure the continuous improvements of hardware and algorithms in the near future. Moreover, it is tailored to Hamiltonian simulation, which is among the most anticipated applications with provable quantum advantage in physics and a building block in many other applications.

We test our method on hardware native geometries and the resulting circuits contain only dense layers of R_{ZZ} gates. However, this does not limit its predictive power since all two-qubit gates are eventually transpiled to the same hardware-native two-qubit gate. One can therefore directly transfer results in terms of two-qubit-gate depth to the simulation of more complicated models. Nonetheless, future research could devise more varied models exhibiting universal behavior that could be used analogously to the KZ scaling. For instance, circuits with interleaved two-qubit gates of different kinds that do not commute with each other such that they cannot be arranged in a dense layer of gates, as for example encountered in fermionic models. Furthermore, our method could be used to select best-qubit subsets. By measuring all nearest-neighbor $\sigma_i^z \sigma_j^z$ correlators on a given quantum

processor, the defect densities of different qubit-subsets can be reconstructed in post-processing. For example, computing the density of defects for all qubit-subsets of size N in this way would allow selecting the subset that best matches the KZ scaling. Moreover, the known finite-size scaling regimes for large annealing times could one day be used to benchmark very deep quantum circuits once they become accessible with advanced EMS techniques or, eventually, quantum error correction (QEC).

Our benchmark extends beyond quantum many-body simulations to quantum optimization. We observe a clear correlation between the threshold number of Trotter steps before the onset of decoherence, identified using the KZ scaling, and the optimal depth when using digitized QA for combinatorial optimization. We demonstrate that, counter-intuitively, the time step should indeed be chosen at a value $\gtrsim 1.0$, resulting in significantly improved residual energy values after annealing. This means in practice that digitized QA is a very competitive quantum optimization framework as it (i) avoids a classical optimization loop and (ii) greatly reduces the runtime of QAOA [81], avoiding the costly iterative optimization, affected by hardware and shot noise [75, 82]. More generally, our results suggest that current hardware with simple EMS may support variational ansatz (for a similar class of Hamiltonians) comprising about ten Trotter-circuit layers. Our results seem to be robust against several instances of disorder with varying minimum spectral gaps as well as on systems of different sizes and connectivities. Nonetheless, future work should aim at exploring other settings such as solving dense graphs [73].

In introducing this benchmark, we report some of the largest-scale digital quantum simulations as of today [14, 83, 84]. Compared to Ref. 14, we move closer to a physical system by incorporating Trotter error and time-dependent, general two-qubit gate angles, requiring a full gate decomposition of the R_{ZZ} gate into hardware native two-qubit gates. However, we do not introduce sophisticated EMS such as probabilistic error amplification, which could be a goal of future work.

Finally, we emphasize that the purpose of the paper is not to claim direct quantum advantage with the featured experiments, including the optimization demonstration. Rather, the benchmarks introduced here will be instrumental to verify future quantum simulations on sufficiently large hardware, beyond the reach of approximate classical methods.

Data Availability

The numerical data that support the findings of this study are available from the corresponding authors upon reasonable request.

Code Availability

The relevant scripts of this study are available from the corresponding authors upon reasonable request.

Acknowledgments

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Appendix A: Error mitigation and suppression

Error suppression refers to methods that actively reduce errors at the circuit level, while error mitigation refers to methods that invert errors in post-processing. We employ some of the most established techniques and provide brief introductions to each one of them in this appendix. More detailed descriptions can be found in the respective references.

1. Readout error mitigation

We employ two methods to mitigate readout errors. When expectation values are evaluated directly, i.e., through QISKIT’s Estimator primitive without evaluating single-measurement bitstrings, twirled readout error mitigation (TREX) is used [66]. TREX twirls the readout with X gates and averages a measured expectation value over these twirls. It can therefore only mitigate readout errors in expectation values, and not on individual bitstrings. That is why, for optimization problems, where individual bitstrings are sampled and processed (with QISKIT’s Sampler primitive), we use matrix-free measurement mitigation (M3) instead of TREX [67].

2. Dynamical decoupling

DD is an error suppression technique that inserts quantum gate sequences during qubit idle times. DD sequences are designed to remove certain system-environment interactions. There exist a plethora of pos-

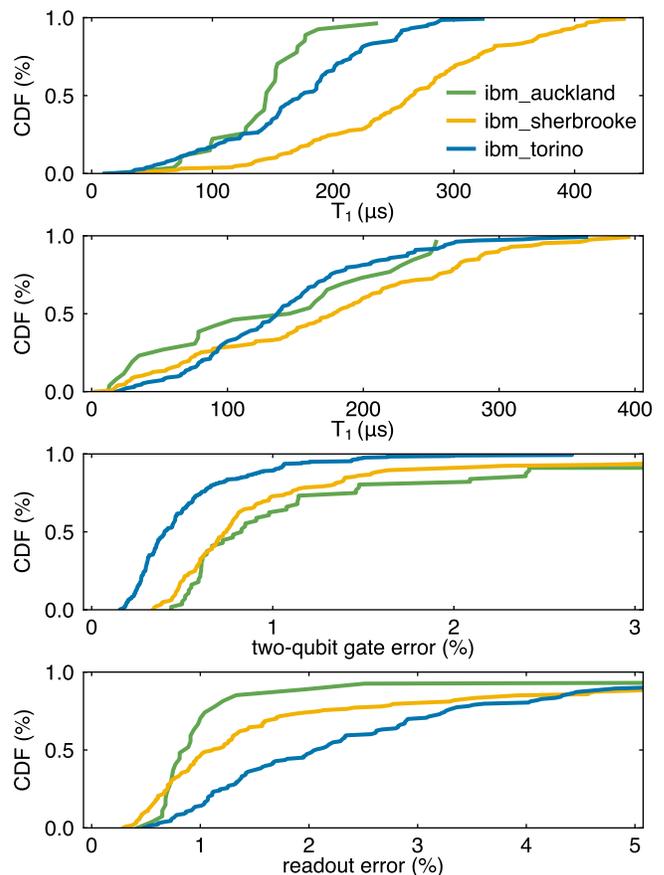


FIG. 6. **Backend Properties.** Cumulative distribution functions of the decoherence times T_1 and T_2 , two-qubit gate and readout errors for the three devices used in this work, *ibm_torino*, *ibm_sherbrooke*, and *ibm_auckland*.

sible DD sequences canceling different errors or canceling errors to different orders [85]. In all experiments with DD, we used a staggered XY4 sequence [68], $Y_0\tau Y_1\tau X_0\tau X_1\tau Y_0\tau Y_1\tau X_0\tau X_1\tau$, with Y_i acting on qubit i and τ being a delay duration. The XY4 = $Y\tau X\tau Y\tau X\tau$ sequence universally cancels all single qubit interactions up to first order. By staggering them, i.e., introducing a relative shift between the sequences on neighboring qubits, we also cancel static ZZ cross-talk [68].

3. Pulse-efficient transpilation

By default, parameterized two-qubit gates such as $R_{ZZ}(\theta)$ are transpiled to a parameterized single-qubit $R_Z(\theta)$ sandwiched between two maximally entangling, hardware-native two-qubit gates. However, if the backend exposes to the user ECR gates as underlying or being its native two-qubit gate and allows for pulse-level access, such gates can be transpiled to significantly shorter final pulse sequences than obtained with standard transpilation. This leads to an overall reduction of the circuit duration. Details can be found in [69] but, in essence,

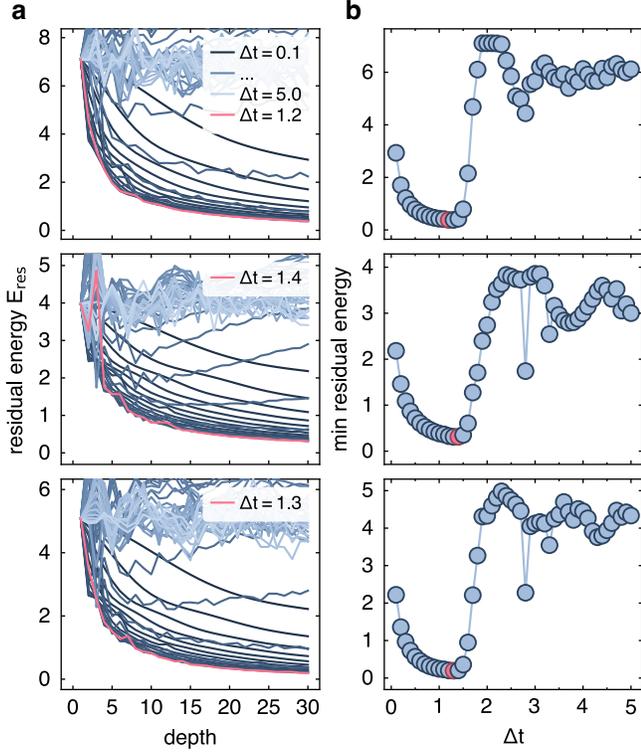


FIG. 7. **Statevector simulations of the residual energy dependence on time step and spectral gap.** **a** Residual energy obtained from statevector simulations of QA with fixed time steps $\Delta t \in \{0.1, \dots, 5.0\}$ as a function of circuit depth, i.e., number of time steps. Each row corresponds to the respective spectrum in Fig. 4. **b** Minimum residual energy from **a** as a function of the time step with fixed depth, i.e., each point corresponds to the minimum over one curve in **a**.

this is achieved by scaling the area of the ECR pulses as a function of the gate parameter θ . In our application, having time-dependent annealing schedules, two-qubit gate parameters start off being small at the beginning of our Trotter circuit and grow towards the end. For our circuits, pulse-efficient transpilation yields a reduction in pulse duration of $\sim 40\%$ on average.

When the gate angle and the corresponding pulse area become so small that not only the pulse width but also its amplitude are adjusted, a fine amplitude calibration becomes necessary [70]. This is due to non-linearities in the cross-resonance gate with respect to pulse amplitude.

Appendix B: Hardware properties and qubit selection

For completeness, we report the decoherence times T_1 and T_2 , the two-qubit gate error, and the readout error as reported for the quantum processors on which we execute the circuits, see Fig. 6. These properties were accessed on 13th February 2024 for `ibm_torino`, on 22nd

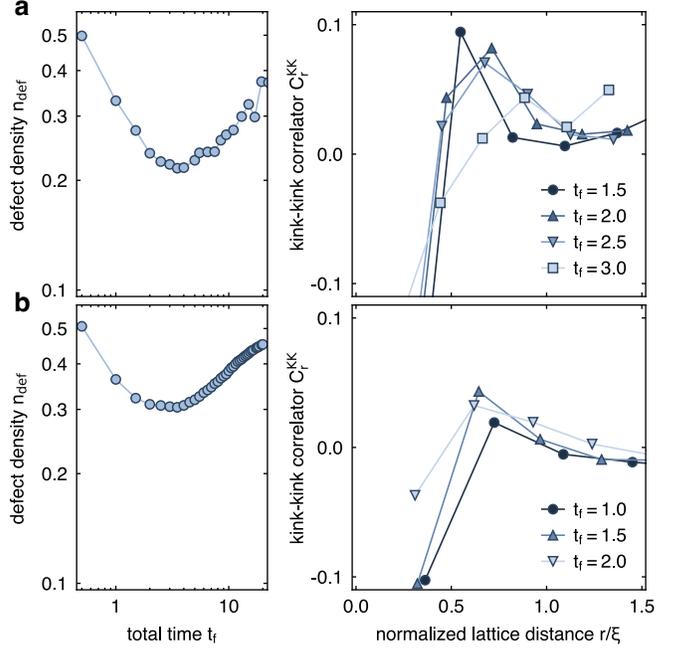


FIG. 8. **Kink-kink correlation functions for different final annealing times t_f .** **a** Density of defects (left) for a periodic 12-qubit chain on `ibm_auckland` using REM and pulse-efficient transpilation and corresponding kink-kink correlators (right). **b** Density of defects (left) of an open 100-qubit chain on `ibm_sherbrooke` using no EMS and corresponding kink-kink correlators (right).

February 2024 for `ibm_sherbrooke`, and on 6th November 2023 for `ibm_auckland`. They are indicative of the device’s performance of when the corresponding experiments in the main text were executed, even though the data reported in the main text were gathered on several different days The 100-qubit line in Fig. 2 was chosen by computing the cumulative two-qubit gate error along all 100-qubit lines on the respective processor and choosing the one with the smallest error.

Appendix C: Quantum annealing with very large time steps

Here, we confirm that the optimal time step for digitized QA for optimization is $\Delta t > 1$ through ideal statevector simulations. Fig. 7 shows the results for the same systems as in Fig. 4 from the main text, that is, instances of disordered couplings $J_{ij} \in [-1, 1]$. When considering a fixed number of time steps or circuit layers, the minimum residual energy obtained from up to 30 time steps decreases with growing time step size up to an optimal time step $1.2 < \Delta t < 1.4$ (depending on the system), before sharply increasing, see Fig. 7. Increasing the time step even further does not yield any benefit whatsoever and, since it induces significant algorithmic errors, results in randomly fluctuating residual energies with increasing

circuit depth.

Appendix D: Kink-kink correlator

Since the KZ scaling of the density of defects could be explained classically [86], we investigate here the correlation between different defects in spin chains after digitized quantum annealing, also termed kink-kink correlation in the literature [30]. Given uniform couplings J , the solution after annealing is ferromagnetic. In this setting, defects are misalignments of spins on edges i between lattice sites, and the correlator between defects i and $i+r$

is defined as

$$C_r^{\text{KK}} = \frac{1}{N_{e,r}} \sum_{i=1}^{N_{e,r}} \frac{\langle K_i K_{i+r} \rangle - n_{\text{def}}^2}{n_{\text{def}}^2}, \quad (\text{D1})$$

where $K_i = 1 - \sigma_i^z \sigma_{i+1}^z$ measures whether there is a defect, i.e. a spin-flip, between sites i and $i+1$, and $N_{e,r}$ is the number of edges on the graph between edges i and $i+r$.

Fig. 8 shows the density of defects (left) of annealing a periodic 12-qubit chain on `ibm_auckland` (a) using REM and pulse-efficient transpilation and of a 100-qubit chain on `ibm_sherbrooke` (b) using no EMS. The corresponding kink-kink correlators for different t_f are shown in the respective right panel as a function of the normalized lattice distance r/ξ with $1/\xi = n_{\text{def}}$. The positive peaks between $r/\xi = 0.5$ and 1.0 imply quantum fluctuations responsible for the defect production.

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