Verification of the Quantum Jarzynski Equality on Digital Quantum Computers

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The quantum Jarzynski equality and the Crooks relation are fundamental laws connecting equilibrium processes with nonequilibrium fluctuations. While they are well established theoretically and also experimental realizations for simple few-body systems already exist, a verification in the quantum many-body regime is still missing. Here, we present results for nonequilibrium protocols in systems with up to sixteen interacting degrees of freedom obtained on trapped ion and superconducting qubit quantum computers, which verify the quantum Jarzynski equality and the Crooks relation in the many-body regime. To achieve this, we overcome present-day limitations in the preparation of thermal ensembles and in the measurement of work distributions on noisy intermediate-scale quantum devices. We discuss the accuracy to which the Jarzynski equality holds on different quantum computing platforms subject to platform-specific errors. Our analysis reveals a novel dissipative nonequilibrium regime, where a fast unitary drive compensates for dissipation and restores the validity of Jarzynski’s equality.

I. INTRODUCTION

More than a century after the foundations of thermodynamics and equilibrium statistical mechanics have been laid, the field of nonequilibrium physics remains an area of active research. The study of how macroscopic properties arise from microscopic quantum dynamics, initiated the development of quantum thermodynamics [1–3]. Significant breakthroughs on the theory side include the widely-applicable eigenstate thermalization hypothesis [4–8], and a handful of interesting cases of its violation [9–11]; at the same time, ongoing experimental progress made it possible to cool down systems to temperatures dominated by quantum over thermal fluctuations [12–15]. Despite this progress, we still lack a comprehensive theoretical framework or a complete set of principles to describe macroscopic phenomena in nonequilibrium physics.

A remarkable achievement in the field is the Jarzynski equality [16, 17]. It establishes a mathematical relation between the work $W$ applied in a time dependent process, and the free energy difference $\Delta F$ between the initial and final thermal ensemble:

$$\langle e^{-\beta W} \rangle_{P(W)} = e^{-\beta \Delta F} \iff \ln \langle e^{-\beta W_{\text{diss}}} \rangle_{P(W)} = 0,$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature with $k_B$ the Boltzmann constant, and $W_{\text{diss}} = W - \Delta F$ is the dissipated work done during the process; the average $\langle \cdot \rangle_{P(W)}$ is performed over the work distribution $P(W)$ obtained from repeated applications of the protocol. Remarkably, Eq. (1) holds for any nonequilibrium protocol without restrictions and for close-to-equilibrium processes it reduces to the well-known fluctuation-dissipation theorem [16].

The classical Jarzynski equality was verified in numerous experimental realizations, ranging from stretching of single molecules [18, 19] to mechanical systems [20], optical tweezers [21], and electronic systems [22].

For quantum systems, a difficulty arises with defining a measurable work operator [23, 24]. Nevertheless, for closed quantum systems, Jarzynski’s equality was extended [25–27] by defining the work $W$ as the difference between the final and
the initial energy:

\[ W = E^f - E^i. \]

(2)

Progress in quantum simulation has facilitated the experimental verification of Eq. (1) with trapped ions [12, 28], cold atoms [29], nuclear magnetic resonance (NMR) experiments [30], nitrogen-vacancy (NV) centers [31], and superconducting qubits [32]. Recently, the quantum Jarzynski equality was also employed to extract approximate free energy differences in two- or three-qubit systems using minimally entangled typical thermal states [33]. Yet, all these experiments were performed only for single-, two-, and three-particle systems; thus, an experimental verification in the quantum many-body regime is still missing. Closing this gap becomes crucial in the light of the rapid development of quantum technologies [34–36], pulling us into the many-body regime. The verification of Jarzynski’s equality in a system of many interacting quantum degrees of freedom represents a natural test for the validity of the laws of quantum thermodynamics in closed systems, on the one side, and the utility of modern quantum simulators to reveal and scrutinize fundamental principles of nature, on the other.

However, the many-body regime poses a number of formidable challenges and limitations. Although Eq. (1) has been verified in composite classical systems as complex as molecules, their dynamics is effectively governed by only a few collective degrees of freedom (e.g., a couple of rotational or vibrational modes). Following Refs. [37, 38], we consider systems of \( L \geq 8 \) spin-1/2 particles to be quantum many-body systems.

In the many-body regime (i.e., for many interacting degrees of freedom), the work distribution broadens linearly with system size, which demands an exponentially large number of measurements in order to estimate the left-hand-side of Eq. (1). Moreover, for quantum systems, further challenges arise: First, work fluctuations are not a measurable observable in quantum mechanics [23]. Hence, testing the quantum Jarzynski equality presumes the ability to measure in the energy eigenbasis, which requires a complete control over the quantum many-body system; this is particularly difficult in practice since many-body eigenstates are typically volume-law entangled in real space. Second, preparing a quantum many-body system in a close-to-perfect thermal state is quite demanding, and often comes with a substantial overhead of resource costs [39, 40]. For these and related reasons, the quantum many-body regime remained beyond the scope of previous works.

Here, we overcome the aforementioned limitations and push the capabilities of quantum simulation beyond the present-day state-of-the-art. In a simulation on digital quantum computers, we verify Jarzynski’s equality for up to \( L = 16 \) qubits in a system of strongly interacting spins governed by the transverse field Ising model and subject to a nonequilibrium protocol. Unlike earlier experiments [12, 28, 30, 33], we do not use a parametric quench, but a protocol of random entangling gates instead. We further demonstrate the validity of the quantum Crooks relation [41] for \( L = 8 \) qubits—an infinitesimal version of Jarzynski’s equality—which, due to its higher computational demand in the quantum regime, had hitherto only been tested for a single two-level system [30, 42].

The complete control over interactions between qubits, together with the ability to perform repetitive measurements on the entire system, make near-term quantum devices a particularly suitable platform to tackle this verification task. We carry out our quantum simulations on four different platforms based on two quantum computing architectures: superconducting qubits (IBM, Rigetti) and trapped ions (IonQ, Quantinuum). We propose Jarzynski’s equality as a new probe to single out dissipation in present-day quantum computers.

In contrast to many common approaches [39, 40, 43–45], we prepare the thermal initial state of the transverse field Ising model without the overhead of using ancilla qubits, using a modification of a protocol proposed in Ref. 46 to include mid-circuit measurements; this allows us to reach system sizes an order of magnitude larger compared to previous studies. We compare the accuracy of our results with the relaxation times on ibm_guadalupe, and identify a novel regime of nonequilibrium qubit dynamics: in there Jarzynski’s equality holds better than one part in ten, even in the presence of accumulating dissipation effects, so long as the execution time of gates is short compared to the thermal qubit relaxation time [so-called \( T_1 \)]. In fact, we find that the nonequilibrium protocol improves the results in comparison to a pure dissipation process.

II. QUANTUM JARZYNSKI EQUALITY AND CROOKS RELATION

Let us recall the derivation of the quantum Jarzynski equality [25, 27]. Consider a system described by a Hamiltonian \( H_t \) with eigenstates \( H_t | m^t \rangle = E^t_m | m^t \rangle \), coupled to a thermal reservoir of inverse temperature \( \beta \). The system is thus described by a thermal ensemble with the density matrix

\[
\rho = Z_t^{-1} \sum_m e^{-\beta E^t_m} | m^t \rangle \langle m^t | ,
\]

where

\[
Z_t = \sum_m e^{-\beta E^t_m} \text{the partition function. We now decouple the system from the reservoir, and let it evolve according to a dynamical process \( U \) (unitary or non-unitary). At the end of this process, the instantaneous final Hamiltonian \( H_f \) of the system has eigenstates \( H_f | n^f \rangle = E^f_n | n^f \rangle \). We denote by \( K_{m \rightarrow n} \) the transition probability from the initial eigenstate \( | m^t \rangle \) to the final eigenstate \( | n^f \rangle \).

The transition probabilities for the dynamical process satisfy the following two sum rules:

\[
\sum_m K_{m \rightarrow n} = 1, \quad \forall m, \quad \text{and} \quad \sum_n K_{m \rightarrow n} = 1, \quad \forall n. \tag{3}
\]

The left-hand equality reflects the conservation of probability. The right-hand sum rule is less obvious and implies the so-called double-stochasticity of the matrix \( K_{mn} \); this condition is fulfilled for unitary dynamics \( K_{m \rightarrow n} = | \langle n^f | U | m^t \rangle |^2 \), but is also conserved throughout evolution in the presence of additional decoherence noise [28]. On the contrary, dissipative noise violates the right-hand sum rule condition [28].

Using these definitions, we can now prove the quantum
Jarzynski equality for the process introduced above:
\[
\left\langle e^{-\beta \Delta W} \right\rangle_{P(W)} = \frac{1}{Z_i} \sum_{m,n} e^{-\beta E^f_n} K_{m-n} e^{-\beta W_{nm}}
\]
\[
= \frac{1}{Z_i} \sum_{m,n} K_{m-n} e^{-\beta E^f_n} = \frac{1}{Z_i} \sum_n e^{-\beta E^f_n}
\]
\[
= \frac{Z_f}{Z_i} = e^{\beta \Delta F},
\]
where we used \( W_{nm} = E^f_n - E^i_m \) according to Eq. (2) in the second line, the double-stochasticity of \( K_{m-n} \) in the third line, and the definition of free energy \( F_1 = -\beta \ln Z_i \) in the last line. We note that Jarzynski’s equality imposes no restrictions on the initial and final Hamiltonians; in particular, they need not be identical.

There exists an infinitesimal (i.e., work-resolved) version of Jarzynski’s equality, called the Crooks relation [26, 41]. The Crooks relation states that
\[
P_F(W) = e^{\beta(W-\Delta F)}.
\]
Here \( P_F(W) \) denotes the probability of extracting an amount of work \( W \) for a given (so-called forward) process and \( P_R(-W) \) for the reverse (or backward) protocol, which can be expressed as
\[
P_F(W) = \frac{e^{-\beta E^f_n}}{Z_i} K_{m-n} \bigg|_{E^i_m - E^f_n = W},
\]
\[
P_R(-W) = \frac{e^{-\beta E^i_n}}{Z_f} K_{m-n} \bigg|_{E^i_m - E^f_n = -W}.
\]

The Jarzynski equality follows by rearranging the Crooks relation, and integrating it over the work \( W \).

### III. SIMULATION ON QUANTUM COMPUTERS

As already pointed out in the introduction, a quantum simulation of Jarzynski’s equality in the many-body regime faces some restrictive challenges.

First of all, the work distribution requires the measurement of initial and final eigenenergies [23], cf. Eq. (2). At the moment, this is only feasible for a suitable choice of the initial and final Hamiltonians, and requires a complete control over the many-body system, including the ability to measure in their respective eigenbases.

We emphasize that the ability to apply general unitary transformations is a distinctive feature of digital quantum computers. In contrast, this is not possible, in general, for other experimental platforms, e.g., cold atom systems [47]; at present, this renders obtaining quantum work distributions in the many-body regime elusive on such platforms.

Second, the verification of Eq. (1) requires the preparation of an initial thermal ensemble. Most approaches for Gibbs state preparation require an overhead of ancilla qubits [39, 40, 43–45]. This makes the use of thermal states in the many-body regime difficult for the current generation of noisy intermediate-scale quantum (NISQ) devices.

Finally, the exponentially growing Hilbert space dimension (in the number of qubits \( L \)) requires an exponential number of projective measurements to approximate the extensive free energy difference \( \Delta F \approx L \). This occurs due to an increasing width of the work distribution \( P(W) \) with system size; it becomes enhanced in the case of generic nonequilibrium protocols which create long tails in the work distribution [48, 49].

In the following, we describe in detail how we tackle each of these challenges. In Sec. III A, we explain our choice for the initial and final Hamiltonians. Section III B elucidates our choice of nonequilibrium protocol, which is summarized diagrammatically in Fig. 2.

In the following we work in units such that \( k_B = 1, \hbar = 1 \).

#### A. Choice of initial and final Hamiltonian

Jarzynski’s equality depends neither on the specific form of the initial or final Hamiltonians, nor on the protocol we evolve the state with. However, a suitable choice of these ingredients is necessary to address the above mentioned challenges, and enables the verification using a simulation on a quantum device in the many-body regime.

##### 1. Initial and final Hamiltonian

Notice that determining the exponentiated work distribution requires measuring the initial and final energy, i.e., two point measurements [23]. In general, this can be achieved by applying a unitary transform to switch to the energy eigenbasis, which is equivalent to diagonalizing the initial and final Hamiltonian, respectively. For generic systems, this requires a circuit of least polynomial depth in the number of qubits \( L \), using a quantum phase estimation algorithm [50]. However, for systems equivalent to free fermionic models, shallow circuits increasing logarithmically with system size suffice [46]. Apart from this practical restriction, the validity of Eq. (1) imposes no further restrictions on the choice of initial and final Hamiltonians. Thus, we choose the initial Hamiltonian to be the transverse field Ising model with periodic boundary conditions [51].

\[
H_i = \sum_{\ell=1}^L \sigma_\ell^x \sigma_{\ell+1}^x + \sum_{\ell=1}^L \sigma_\ell^z.
\]

This system is integrable and can be mapped to free fermions through a Jordan-Wigner transformation. It can be diagonalized using a shallow circuit as described in Ref. 46.

The inverse transformation from the single-particle eigenmodes to the spin basis includes a Bogoliubov transform and a fermionic Fourier transform, which constitute part (B) of our circuits increasing polynomially in the number of qubits \( L \), using a quantum phase estimation algorithm [50]. However, for systems equivalent to free fermionic models, shallow circuits increasing logarithmically with system size suffice [46]. Apart from this practical restriction, the validity of Eq. (1) imposes no further restrictions on the choice of initial and final Hamiltonians. Thus, we choose the initial Hamiltonian to be the transverse field Ising model with periodic boundary conditions [51].

\[
H_i = \sum_{\ell=1}^L \sigma_\ell^x \sigma_{\ell+1}^x + \sum_{\ell=1}^L \sigma_\ell^z.
\]
As a final Hamiltonian, we chose the simple Hamiltonian

$$H_t = \sum_{\ell=1}^L \sigma_\ell^z,$$  \hspace{1cm} (9)

which is already diagonal in the computational basis, such that measurements in the eigenbasis of $H_t$ are straightforward. Overall, the choice of the initial and final Hamiltonians, which are either already diagonal in the computational basis, or a circuit is known to diagonalize them in practice, enables us to perform a two-point measurement protocol for determining the work; this is essential to measure the left-hand side of the Jarzynski equality, cf. Eq. (1).

The partition function for a system of non-interacting fermions can be written as:

$$Z_i = \sum_{\omega_1,..,\omega_L} \omega_1 \omega_2 \cdots \omega_L e^{\beta \omega_1 + \beta \omega_2 + \cdots + \beta \omega_L}.$$

with the energies $\omega_k$ are defined in App. A; the energy offset is given by $E_c = 1 - \sqrt{2}$. The partition function is therefore given by

$$F_i = E_c - \frac{1}{\beta} \sum_{k=-L/2+1}^{L/2} \ln(1 + e^{-\beta \omega_k}).$$  \hspace{1cm} (11)

The free energy of the final Hamiltonian is

$$F_f = -\frac{L}{\beta} \ln \left(2 \cosh \left(\frac{\beta}{2}\right)\right).$$  \hspace{1cm} (12)

In order to validate Eq. (1), it is therefore sufficient to concentrate on obtaining the exponentiated work distribution on the left-hand side.

2. **Gibbs ensemble preparation**

To test the Jarzynski equality, we need to prepare a thermal ensemble governed by the chosen initial Hamiltonian on the quantum simulator. While this is a hard task on quantum devices in general, since energy eigenstates are not accessible, the transformation of the Ising model into a model of many non-interacting fermions allows us to use the initial energy measurement to prepare a thermal ensemble.

The density matrix for a system of non-interacting fermions can be written as:

$$\rho_i = \frac{1}{Z_i} \sum_{m} e^{\beta E_m} |m\rangle \langle m|$$

$$= \frac{1}{Z_i} \bigotimes_k \left( e^{-\beta \omega_k} |1\rangle_k \langle 1|_k + |0\rangle_k \langle 0|_k \right).$$  \hspace{1cm} (13)

Here $\omega_k$ denotes again the energy of the single-particle eigenvalues. Starting from the product state $|0\rangle^\otimes L$, the Gibbs ensemble for this system is obtained by applying a rotation gate $U_k$ on each qubit of the form

$$U_k \equiv U(\theta_k) = \begin{pmatrix} \cos \theta_k & -\sin \theta_k \\ \sin \theta_k & \cos \theta_k \end{pmatrix},$$  \hspace{1cm} (14)

with $\theta_k$ chosen as,

$$\sin^2 \theta_k = \frac{e^{-\beta \omega_k}}{1 + e^{-\beta \omega_k}},$$  \hspace{1cm} (15)

and a subsequent measurement of all spins in the computational basis (Fig. 2 A). After this measurement, we apply a unitary transform to get the thermal ensemble in the original spin basis, as shown in Fig. 2 B.

3. **Midcircuit measurements vs. classical presampling**

Our approach requires performing mid-circuit measurements on a quantum device. Unfortunately, this is not feasible
on all present-day quantum computing platforms. Wherever this is not the case, we use classical presampling, as is also done in previous proposals [46] and related recent works [31, 53]. To do so, we replace section (A) in our circuit (Fig. 2) by the preparation of a randomly chosen eigenstate, with probability equal to its Boltzmann weight. Since the single-particle representation is already diagonal in the computational basis, this can be achieved by applying NOT-gates to the corresponding excited eigenmodes. At the end, each eigenstate \( \ket{m_i} \) is prepared \( M_i \geq 0 \) times, with \( \sum M_i = M \) the total number of measurements.

However, at the end we want to perform a quantum simulation. In light of that, we avoid classical presampling, whenever possible and stick to midcircuit measurements for the largest system sizes \( L = 16 \).

After discussing the issues of measuring work and thermal state preparation, we move on to partially address the remaining points concerning the exponential scaling of shots and free energy differences.

### B. Nonequilibrium protocol

In contrast to previous experiments, the local control over qubit interactions offers a significant freedom in the choice of nonequilibrium protocol, cf. part (C) of our circuit in Fig. 2.

Due to the nature of gates on digital quantum computers, we choose a circuit whose dynamics does not describe a parametric deformation between the initial and final Hamiltonians. This allows us to explore nonequilibrium regimes away from adiabatic ramps, for which Jarzynski’s equality reduces to the fluctuation-dissipation theorem [12].

Instead, in our digital quantum simulations, we apply a protocol consisting of \( k \)-local sequential blocks, as shown in Fig. 2(C). Each block consists of a layer of single-qubit Haar random unitary gates, followed by a sequential layer of CNOT-gates. In comparison to pure Haar random circuits, our circuit allows for a more native and shallow implementation on NISQ devices; moreover, \( L - 1 \) blocks are sufficient to build up bipartite von Neumann entanglement in the system close to the Page value [54], as we demonstrate in a classical emulation in App. B.

The choice of such a circuit renders the work distribution close to a Gaussian with increasing system sizes, cf. App. B. As a consequence, the effect of anomalous rare trajectories, which might dominate the averaged exponentiated work distribution [48, 49], is suppressed. This reduces the number of required measurements to estimate Eq. (1), such that accurate results for \( L = 16 \) qubits with a realistic number of quantum measurements can be achieved.

In order to determine the final energy, and with it, the work, we perform up to \( 2^{24} \) measurements on superconducting quantum computing architectures and between \( 2^{12} \) (Quantinuum) and \( 2^{16} \) (IonQ) measurements on trapped ion platforms. The reason for the smaller number of measurements on trapped ion devices is the higher cost of the quantum simulation, which restricts us to use less data points.

Overall, the choice of the protocol and the specific features of a quantum computer allow us to at least partially address the exponential scaling of the number of required measurements.

Last, it is curious to note that the separation of parts (B) and (C) in our protocol [Fig. 2] is somewhat arbitrary. On the one hand, part (B) belongs naturally together with part (A) in a thermal state preparation subprotocol. On the other, we can interpret part (B) as part of the nonequilibrium protocol (C) applied to the system. Since Jarzynski’s equality holds for arbitrary protocols, equilibrium or nonequilibrium, the accuracy of implementation of part (B) is not crucial for the accuracy to which we verify Jarzynski’s equality. Note that this does not compromise the many-body character of our circuit: indeed, our circuit fully explores all degrees of freedom of the many-body system, and populates generic (i.e., non-product) states in the many-body Hilbert space, since the entanglement created by the circuit reaches the maximal Page value, cf. Fig. 9.

### IV. COMPARISON OF DIFFERENT NISQ ARCHITECTURES

Before we present our results, we give a brief overview of the different quantum computing platforms, the noise they are affected by, and the impact of the latter on the validation of Jarzynski’s equality on various quantum devices.

#### A. NISQ architecture characteristics

In order to test the effect of different noise types, we run our circuits on five different devices using two different architectures: superconducting qubits (ibm_perth, ibmq_guadalupe and Rigetti Aspen-11), and trapped ion platforms (Quantinuum H1 and an 11-qubit system of IonQ). We extract the exponential of the work, Eq. (2), to validate the Jarzynski equality, cf. Eq. (1). As mentioned above the latter is valid also in the presence of noise which does not violate double-stochasticity, and is only sensitive to dissipative errors that violate the second sum rule in Eq. (3).

The quality of qubits is often measured by means of the average gate times \( T_2 \) and the relaxation times \( T_1 \) and \( T_2 \). The timescale of dephasing errors, \( T_2 \), is not relevant for our purposes, since depolarizing errors do not violate double-stochasticity. Only the thermal relaxation time \( T_1 \) or, more concretely, the ratio \( q = T_2 / T_1 \) matters, as it sets the decay rate for excited states, cf. Sec. V. While the two-qubit fidelities for all architectures fall between 95% and 99.5%, the \( q \)-factor depends strongly on the underlying architecture.

The two-qubit gate time for IonQ-devices is \( T_2 \approx 200 \mu s \), and the relaxation time \( T_1 \sim 10^7 \mu s \), resulting in a factor \( q_{\text{IonQ}} \sim O(10^5) \). On the other hand, the timescale for IBM-platforms are \( T_2 \approx 400 \text{ns} \), \( T_1 \sim 160 \mu s \), yielding \( q_{\text{IBM}} \sim 400 \). We anticipate, therefore, to recover Jarzynski’s equality significantly more accurately on trapped ion than on superconducting platforms.
data for different inverse temperatures with a total of classical postprocessing. In this way, we are able to extract information about the compiled circuit and gate times. The accuracy of the results on ibmq_guadalupe is comparable to that on the trapped ion device IonQ.

**TABLE I.** Accuracy of the Jarzynski equality for $\beta = 0.7$, executed on different devices for an extension of the protocol from Fig. 2 to $L = 8$ qubits. The case for mid-circuit measurements is shaded in grey. The values for the runtimes on IonQ and Rigetti are extrapolated, using rough estimates for the measurement errors and their impact on the validity of Jarzynski’s equality.

The errors for the IonQ, Rigetti and IBM devices are within 2% to 5%, even for large values of $\beta$ and $L = 8$ qubits. Note that the theory predicted value from Eq. (1), $\ln \langle e^{-\beta W_{\text{mix}}} \rangle_{P(W)} = 0$, does not fall within the error bars for the superconducting architectures—a direct manifestation of dissipative effects.

Even if deviations from Jarzynski equality Eq. (1) are not detectable with the current experiment, a closer look reveals that the measurement process itself is a dissipative process in this case: our quantum simulations reveal that excited qubits are detected in the ground state with a probability of roughly 1%. This process violates the second sum rule in Eq. (3), and thus leads to a weak violation of the quantum Jarzynski equality. As discussed in App. C, our simulations reveal a means to detect the readout error as residual deviation in the limit of infinite measurements.

It is also insightful to compare the deviation from Eq. (1) with and without error-prone mid-circuit measurements on a IBM quantum device. In the case of $L = 8$ qubits, the error is increased by almost a factor of 2 due to the first measurement, as is shown in Table I. This already shows that most of the deviation from the theoretical prediction is due to the measurement process.

On Rigetti Aspen-11, we found it was essential to disable “fencing” to obtain quality results on par with other devices. Fencing makes two-qubit gates executed sequentially, even when acting on different qubits within the same circuit layer. While this reduces crosstalks and increases the fidelity of the individual operations, it leads to circuits with a longer execution time, making relaxation effects through $T_1$ more prominent.

**Runtime and resource cost.**—Regarding the execution time,
note that different physical platforms have different run times. In the case of superconducting qubits, gates are implemented as a sequence of microwave pulses, where the average duration of each such gate is of the order of 10 ns to 100 ns [55]; thus, the overall circuit duration for \( L = 8 \) qubits is of the order of 50 \( \mu s \). In the case of trapped ions, gates are implemented via two-photon Raman processes, with gate times ranging from 10 \( \mu s \) to 100 \( \mu s \) [56]. As a consequence, the execution time for a circuit is also three orders of magnitude longer, which presents a relevant bottleneck for us when increasing the system size or the number of measurement shots.

The use of different architectures also affects the simulation cost. The simulation cost on trapped ion systems is at least 30 times higher than on superconducting qubits, which is caused by the longer circuit evaluation times. This is the major bottleneck we encounter for simulations on trapped ion devices: it limits the number of circuit evaluations to \( 2^{16} \) and the system size to \( L = 8 \) qubits on IonQ, and to 4,000 evaluations on \( L = 4 \) qubit systems on Quantinuum H1, respectively.

**Ability to perform midcircuit measurements**— At the end we want to perform a quantum simulation without any classical presampling. The thermal state preparation introduced in Sec. III A 2 requires the ability to perform midcircuit measurements. From the above platforms, only the IBM and Quantinuum devices are currently capable of performing this task.

Taking the accuracy of the results, the hardware abilities, and the resource cost altogether into account, through the rest of this paper we present results exclusively obtained on the ibmq_guadalupe processor.

### V. VERIFYING JARZYNSKI’S EQUALITY AND CROOK’S RELATION IN THE MANY-BODY REGIME

#### A. Jarzynski relation in the many-body regime

In order to compare results for different system sizes, we choose the case of maximum dissipation to the ground state as a natural scale to quantify deviations from the Jarzynski equality. For this purpose, we define the work done in a purely dissipative decay process, \( \mathcal{W}_{\text{dec}} \), implicitly via the relation:

\[
\begin{align*}
    e^{-\beta \mathcal{E}_{\text{cro}}_{\text{dec}}} &\equiv e^{-\beta (E^{\dagger}-E_{\text{het}})} e^{-\beta \Delta F}.
\end{align*}
\]

Here the bar \( \langle \cdot \rangle \) denotes an average over the initial thermal ensemble. Intuitively, the above equation gives the expected deviation of Eq. (1) when the state decays into the ground state of each qubit with unit probability.

The purely dissipative process causes the maximum possible deviation from the Jarzynski equality in our circuit setup. Thus, we can use it as a reference to quantify the amount of violation. To this end, we define the relative deviation from the theoretical prediction:

\[
\mathcal{E}(\beta) = \frac{\ln \langle e^{-\beta \mathcal{W}_{\text{dec}}} \rangle_{\mathcal{P}(W)}}{\ln e^{-\beta \mathcal{W}_{\text{dec}}}}.
\]

Whenever Jarzynski’s equality holds, we have \( \mathcal{E}(\beta) = 0 \); on the other hand, for a purely dissipative (i.e., maximum-decay) process, \( \mathcal{E}(\beta) = 1 \).

The violation of the Jarzynski equality for \( \mathcal{L}=4, \mathcal{L}=8, \) and \( \mathcal{L}=16 \) qubits is shown in Fig. 4 as a function of inverse temperature. As anticipated, the absolute violation [Fig. 4(a)] grows with increasing the system size. However, the relative deviation \( \mathcal{E} \) [Fig. 4(b)] exhibits only a weak system-size dependence, since the latter is absorbed by the scaling of the denominator, \( \ln e^{-\beta \mathcal{W}_{\text{dec}}} \propto \beta \mathcal{L} \) for small \( \beta \).

Since increasing the system size requires a larger circuit depth through the sub-circuits (B) and (C) [cf. Fig. 2], one could naïvely expect that scaling to large system sizes is quickly hampered by dissipation effects which accumulate with increasing circuit size. However, this appears at odds with the observed behavior in Fig. 4, where we show data up to \( \mathcal{L} = 16 \) qubit chains. Therefore, we now briefly investigate our circuit’s susceptibility to dissipation.

The purely dissipative process leading to the right-hand-side of Eq. (16) can be emulated on a NISQ device by applying a so-called “idle process” [57]: this is a similar process as the...
one described in Fig. 2, but with the circuit parts (B) and (C) replaced by free evolution for a variable duration $t_{idle}$. Hence, the two measurements at the end of circuit part (A) and in part (D) are separated by the idle time $t_{idle}$. Hence, to access the regime of validity of Eq. (16), we have to apply an idle process of time $t_{idle} \gg T_1$.

Figure 5 shows the relative deviation from Jarzynski’s equality for an idle process, as a function of the waiting time $t_{idle}$ for $L=8$ qubits. As expected, for large waiting times $t_{idle} \geq T_1$, $\mathcal{E} \to 1$ reaches the limit of a pure dissipative process. We can now compare the time required to reach the purely dissipative regime with the execution time of the circuit from Fig. 2. Before we do this, notice first that the average dissipation time of ibmq_guadalupe is $T_1 = 118 \mu s$, while the execution time for our circuit [Fig. 2, (A) to (D)] is $T_c = 57 \mu s$ for $L = 8$ qubits; hence $T_c/T_1 \approx 0.48$ [cf. dashed vertical line in Fig. 5].

The relative deviation from Jarzynski’s equality is shown for our circuit as diamonds on the dashed vertical line in Fig. 5. Comparing the deviation values with the dashed idle process, the accuracy of the process from Fig. 4 appears quite striking, since it is an order of magnitude smaller than an idle protocol of the same waiting time, $t_{idle} = T_c$. In fact, the deviation values are comparable to those of the idle process with the smallest idle time investigated, from which we can deduce that the main source of deviations from Eq. (1) originates in part (D) of the protocol.

To sum up, our nonequilibrium circuit has the property of preventing dissipation effects from accumulating, despite increasing circuit execution time; this is, in turn, reflected in Jarzynski’s equality being obeyed to a high degree of accuracy even in the many-body regime of $L = 16$ qubits. We will discuss this observation in more detail in Sec. VI.

![FIG. 5. Relative deviation from Jarzynski’s equality as a function of the waiting time $t_{idle}$ (solid lines), for four different inverse temperatures $\beta$, at $L = 8$. The $x$-axis is normalized by the average waiting time $T_1 = 118 \mu s$. For comparison, the diamonds denote the results for our protocol shown in Fig. 4(b), placed at their respective execution time [dashed vertical line]. The application of gates between the two measurements in the protocol [cf. Fig. 2] improves the accuracy of our results by more than one order of magnitude.](image)

![FIG. 6. (a) Verification of the Crooks relation $\ln \left( \frac{P_F(W)}{P_R(-W)} \right)$ as a function of the work $W$. The color denotes the density of data points, from low (black) to high density (yellow). The cyan line denotes the theoretical prediction and the light green line is a fit $\tilde{\beta}(W - \Delta F)$, with $\tilde{\beta} = 0.94$ for the experimental data points. (b) Same data, but this time the colorbar denotes the minimum probability of the reverse and forward process $P_F(W)$ and $P_R(-W)$ respectively. Optimal fit to a linear function is shown in black, and theory prediction is shown in red. While the overall trend of all points follows the Crooks relation [red line], we see significant energy-dependent deviations from it, presumably caused by the specific design of our reverse and forward process [see text]. The data shown here are for $\beta = 1.0$, $2^{24} \sim 1.7 \times 10^7$ shots and $L = 8$ qubits on ibmq_guadalupe.](image)

### B. Crooks relation in the many-body regime

While Jarzynski’s equality is a statement about work-averaged processes, we can also check to what extent its infinitesimal [or in-sample] version – the Crooks relation $[26, 41]$ [see Sec. II]

$$\ln \left( \frac{P_F(W)}{P_R(-W)} \right) = \beta(W - \Delta F)$$

– holds. To the best of our knowledge, the latter was only tested for two-level systems so far [30, 42].

For a process described by a sequence of unitary gates, and ignoring noise for a moment, the backward process can be implemented in a straightforward way by reversing their order and taking the inverse of each individual gate.

It is important to note that the Crooks relation requires exponentially more measurements than the verification of Jarzynski’s equality, since we need to check whether it holds for each of the $4^L$ possible eigenstate transitions of the process. For this reason, we are limited to $L = 8$ qubits, using $2^{24} \approx 1.7 \times 10^7$ measurements.
The corresponding data for the Crooks relation are shown in Fig. 6a. The validity of the Crooks relation requires that all data points lie on the cyan line, apart from statistical fluctuations arising from a finite number of measurements. Indeed, the data follow the trend predicted by the Crooks relation; the fitted slope of the data $\beta = 0.94$ deviates by 6% from the theoretical-predicted value $\beta = 1$. However, we observe strong fluctuations around the theory prediction; the ratio between occurrences of forward and backward processes in Eq. (5) is up to one order of magnitude larger than predicted by theory. To understand these fluctuations, the datapoints for different pairs of forward and backward processes are shown in Fig. 6 (b).

The transfer matrix according to

$$\mathcal{C} = \begin{pmatrix} C_0 \end{pmatrix}$$

and

$$\mathcal{U} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix},$$

where $\alpha = \text{arctan}(2\sqrt{p})$.

Then the density matrix vector evolves under this unitary matrix according to

$$\hat{\rho} \rightarrow (U \otimes U^\dagger) \hat{\rho},$$

where $\alpha$ denotes complex conjugation. Let us also assume that the excited state has only a finite lifetime $T_1$; thus, we use a single amplitude damping channel [58] to describe this effect.

The time evolution over one period is then given by

$$\mathcal{F}(\rho) = \sum_{i=1}^{2}(\mathcal{K}_i \otimes \mathcal{K}_i^\dagger)(U \otimes U^\dagger)\hat{\rho} \equiv \mathcal{C}\hat{\rho}. \quad (22)$$

The transfer matrix $\mathcal{C}$ is implicitly defined via this process, and has a unique largest eigenvalue $\lambda = 1$ for $p > 0$. The Kraus operators $\mathcal{K}_i$ describing the damping process are given by,

$$\mathcal{K}_1 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \quad \text{and} \quad \mathcal{K}_2 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}. \quad (23)$$

The parameter $p$ is the fraction of the excited state population which decays to the ground state after one application of $C$. It is related to the relaxation time $T_1$ and the gate time $T_g$ via

$$p = 1 - \exp \left( \frac{-T_g}{T_1} \right). \quad (24)$$

Repeating the process $N$ times, the density matrix evolves in the long time limit as

$$\hat{\rho}^{\text{ev}} = \lim_{N \to \infty} \mathcal{F}^N(\rho) = \lim_{N \to \infty} \mathcal{C}^N \hat{\rho} \equiv C_0 \hat{\rho} + O \left( (1 - p)^{\frac{N}{2}} \right), \quad (25)$$

where $C_0$ corresponds to the steady state of the transfer operator $\mathcal{C}$. A simple calculation gives, for $p > 0$,

$$C_0 = \begin{pmatrix} 1/2 + f(p, \alpha) & 0 & 0 & 1/2 + f(p, \alpha) \\ g(p, \alpha) & 0 & 0 & g(p, \alpha) \\ g(p, \alpha) & 0 & 0 & g(p, \alpha) \\ 1/2 - f(p, \alpha) & 0 & 0 & 1/2 - f(p, \alpha) \end{pmatrix}, \quad (26)$$

with

$$f(p, \alpha) = \frac{p \left[ 1 - \sqrt{1 - p} \cos(2\alpha) \right]}{2 \left[ 1 - p + \sqrt{1 - p} \right] \left[ 1 - \cos(2\alpha) \right]}, \quad (27)$$

and

$$g(p, \alpha) = \frac{p \sqrt{1 - p} \sin(2\alpha)}{2 \left[ 1 - p + \sqrt{1 - p} \right] \left[ 1 - \cos(2\alpha) \right]}. \quad (28)$$

Using the definition of the matrix $C_0$, the transition matrix $K$ of this process is given by

$$K = \begin{pmatrix} 1/2 + f(p, \alpha) & 1/2 + f(p, \alpha) \\ 1/2 - f(p, \alpha) & 1/2 - f(p, \alpha) \end{pmatrix}. \quad (29)$$

Comparing this expression with Eq. (3), we can see that the requirements for Jarzynski’s equality are recovered for $f(p, \alpha) = 0$, which is the case at $p = 0$. An expansion of $f(p, \alpha)$ around $p = 0$ gives, together with Eq. (24)

$$f(p, \alpha) = \frac{1}{4}p + O(p^2) = \frac{1}{4} T_g^2 \frac{T_1}{T_1} + O \left( \frac{T_g^2}{T_1} \right). \quad (30)$$

This limit is thus approached in the case of an infinitely fast drive, as can be seen from the relation in Eq. (30). Note that the actual time of the protocol does not matter in this case, since this analysis holds in the limit of infinitely many periods $N \to \infty$. Indeed, there is no obstruction if the protocol time greatly exceeds the relaxation time scale $T_1$.

Although we restricted the analysis to the case of a single qubit with a periodic protocol, our quantum simulations suggest that the underlying physics remains the same for random gates and multi-qubit systems. The relevant physical parameter is $p$, as defined in Eq. (24). The application of single-qubit gates can be seen as a drive applied to the system, which repopulates excited states, and thus compensates for the deviations
from Jarzynski’s equality caused by the dissipation process. This explains why the results of our circuit protocol surpass those of the idle process by one order of magnitude, cf. Fig. 5.

Our toy model is also sufficient to explain the energy fluctuations in the verification of the Crooks relation. To do so, let us again take a closer look at the specific Jarzynski protocol in Fig. 2 and the role of dissipation discussed above. Towards the end of the backward process, gates for the Fourier and Bogoliubov transforms are applied. Their implementation requires many SWAP gates, since only two-qubit operations between neighboring qubits are allowed on IBM devices. On the other hand, almost no single-qubit gates are applied at the end of the reverse process. As a consequence, the part of the drive that compensates for dissipation is weaker in the reverse direction; thus, a larger fraction of reverse processes have the qubit state population decay into low-lying energy states, before they complete. Hence, the forward and backward processes are no longer balanced, and deviations from the Crooks relation become observable.

### VII. DISCUSSION & OUTLOOK

In summary, we proposed a protocol to validate the quantum Jarzynski equality and the Crooks relation in the many-body regime on near-term quantum computing devices, in the presence of different errors.

As a side product, our protocol in Fig. 2 reveals the ingredients of Eq. (1) in a simple way. The quantum Jarzynski equality is a relation between initial and final eigenenergies, and a double-stochastic transfer matrix connecting them. Anything else, including the transformation to a physical basis can be absorbed into the transition process itself. The quantum Jarzynski equality thus probes only the double-stochasticity of the process violated by dissipation, not the accuracy of different parts of the protocol.

We pushed the state of the art for a quantum simulation of Jarzynski’s equality up to 16 qubits, and for the Crooks relation – to 8 qubits, respectively. We compared different quantum architectures and the limitations they pose in the study of nonequilibrium dynamics of thermal quantum systems, including in the presence of intrinsic errors on NISQ devices. While trapped ion platforms show more accurate results in the validation of Jarzynski’s equality, when it comes to simulation cost and time, superconducting platforms scale more favorably to larger system sizes. Hence, restricting our study to the ibmq_guadalupe quantum processor, we managed to reach the largest system size in our quantum simulations.

It is also interesting to compare our results to previous experiments on the quantum Jarzynski equality, cf. Table II. To this end, we first extract the results for the left-hand side of Eq. (1), and the theory prediction of the free energy of the corresponding experiments; then we compute the maximum deviation of an idle process, cf. Eq. (16), which gives us the normalized deviation defined in Eq. (17) for each experiment [cf. Appendix D for details]. The comparison shown in Table II clearly suggest that the accuracy of our results is comparable with most of the earlier experiments; however, we reach an order of magnitude larger system sizes, where quantum many-body effects are pronounced.

Moreover, in contrast to previous experiments, the protocol duration of our circuits is comparable to, or even exceeds, the average dissipation time \( T_I \) of the NISQ devices; therefore, dissipation is no longer negligible. We checked that our results do not depend on the specific choice of randomness in our protocol. Furthermore, we demonstrated that the relative accuracy of our results is almost independent of system size and circuit depth. By employing a fast drive which compensates for dissipation, we thus found a novel regime where the Jarzynski equality holds in an emergent way.

| Experiment | Experimental platform | System size \( L \) | Inverse temperature \( \beta \) | Relative accuracy \( \mathcal{E}(\beta) \) |
|------------|-----------------------|--------------------|-------------------|-------------------|
| This work  | superconducting qubits| 16                 | 0.7               | 0.061(3)          |
| Ref. 33    | superconducting qubits| 3                  | 1.0               | 0.03(1)           |
| Ref. 32    | superconducting qubits| 1                  | 1.0               | 0.02(2)           |
| Ref. 12    | trapped ions: vibrational modes | 1 | 1.13 | 0.02(2) |
| Ref. 28    | trapped ions: two hyperfine levels | 1 | 1.3 | 0.03(9) |
| Ref. 30    | NMR                   | 1                  | 0.15              | 0.17(8)           |
| Ref. 29    | Hyperfine levels of \(^{87}\)Rb | 1 | 1.75 | 0.00(4) |
| Ref. 31    | NV centers            | 1                  | 0                 | 0                 |

TABLE II. Comparison of different experiments for the validation of the quantum Jarzynski equality, using the normalized deviation defined in Eq. (17). The relative accuracy \( \mathcal{E} \) of our simulations is comparable with previous experiments on few-qubit systems. More details for the extraction of the data and the determination of \( \beta \) are provided in the appendix D.
While this observation is interesting on its own, it shows up a promising direction to investigate errors on NISQ devices in new ways: Since Jarzynski’s equality is only sensitive to dissipative noise, it can be used to quantify and single out its effect. Even if simpler protocols to determine the dissipation time $T_1$ of devices exist [58], our approach is tailored to study noise effects on entangled qubits in the many-body regime; this shows promise to refine our understanding of correlated error processes on modern quantum devices. Furthermore, it raises the more general question of whether or not it is possible to find other measurable physical quantities, that are susceptible to specific features of the system-environment coupling.

Finally, in contrast to common approaches [39, 40, 43–45], our protocol points towards an exciting practical direction for preparing thermal ensembles using mid-circuit measurements without the overhead of ancilla qubits. In fact, since the target outcome is not a pure state, the use of non-unitary ingredients appears natural in this setting. In our study, we restricted to Hamiltonians which can be mapped to single-particle systems by using shallow circuits; it is currently an open question whether, to what accuracy, and under which conditions, one could prepare thermal ensembles for more general Hamiltonians.

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Appendix A: Preparation of a thermal distribution for the transverse field Ising model

1. Theory

The transverse field Ising model can be mapped to a non-interacting fermionic Hamiltonian. It is therefore possible to prepare it in a Gibbs ensemble, using the protocol described in Sec. III A 2 and with the help of a unitary transformation between the energy and spin bases of the system. The different transformation steps are explained here in detail, following Ref. [46].

The transverse field Ising model is given by a Hamiltonian

$$H' = \sum_{i=1}^{L} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^{L} \sigma_i^z \sigma_i^z. \quad (A1)$$

We always set $\lambda = 1$ for the simulations in the main text. In order to simplify the realization on a quantum computer, we impose periodic boundary conditions, and add an additional Pauli string to eliminate unwanted terms that appear in the Jordan-Wigner transformation:

$$H = \sum_{i=1}^{L} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i=1}^{L} \sigma_i^z \sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z. \quad (A2)$$

Note that the multi-body term becomes negligible in the thermodynamic limit.

As a first step, we transform the Hamiltonian into fermionic modes using a Jordan-Wigner transform:

$$c_j = \left( \prod_{i<j} \sigma_i^z \right) \frac{\sigma_j^x + i \sigma_j^y}{\sqrt{2}}, \quad c_{-j}^\dagger = \frac{\sigma_j^x - i \sigma_j^y}{\sqrt{2}} \left( \prod_{i<j} \sigma_i^z \right). \quad (A3)$$

This gives the following fermionic Hamiltonian:

$$H = \sum_{i=1}^{L-1} \frac{1}{2} \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i c_{i+1} + c_{i+1}^\dagger c_i^\dagger \right) + \lambda c_i^\dagger c_{i+1}^\dagger. \quad (A4)$$

The wave function can be expressed as

$$|\psi\rangle = \sum_{i_1, \ldots, i_L = 0,1} \psi_{i_1, \ldots, i_L} |i_1 \ldots i_L\rangle$$

$$= \sum_{i_1, \ldots, i_L = 0,1} \psi_{i_1, \ldots, i_L} c_{i_1}^\dagger \ldots c_{i_L}^\dagger |\Omega_N\rangle. \quad (A5)$$

Here $|\Omega_N\rangle$ is the vacuum state, i.e., $c_i |\Omega_N\rangle = 0$. Note that the coefficients of the wave function do not change; thus, the Jordan-Wigner transformation does not add any additional gates to the quantum circuit. However, we have to keep track of fermionic signs when swapping fermionic modes.

The next step is to apply a Fourier transform:

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_{j=0}^{L-1} e^{-\frac{2\pi i k j}{L}} c_j^\dagger, \quad k = -\frac{L}{2} + 1 \ldots \frac{L}{2}. \quad (A6)$$

The Fourier transform for $L = 2^n$ qubits can be achieved with a quantum circuit of depth $\log(L)$. To see why, we split the Fourier transform into even and odd sites:

$$\sum_{j=1}^{L} e^{\frac{2\pi i k j}{L}} c_j^\dagger = \sum_{j'=0}^{L-1} \left( e^{\frac{2\pi i k j'}{L}} c_{2j'}^\dagger + e^{\frac{2\pi i k j'}{L}} c_{2j'+1}^\dagger \right). \quad (A7)$$

The two terms on the right-hand-side independently represent a Fourier transform for $L/2$ fermions. The case $L = 2^k$ is
particularly appealing, since we can keep iterating this step until we end with a Fourier transform of only two fermions, which can be easily implemented using two-qubit gates.

To do so, we need the fermionic swap gate (note the sign structure, green gates in Fig. 7)

\[ f_{\text{SWAP}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad (A8) \]

and the Fourier gates (light blue gates in Fig. 7)

\[ F_k = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{e^{2\pi i k}}{\sqrt{2}} & \frac{e^{\pi i k}}{\sqrt{2}} & 0 \\ 0 & \frac{e^{-2\pi i k}}{\sqrt{2}} & \frac{e^{-\pi i k}}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (A9) \]

In our case, we have to restrict to \( L \leq 16 \), due to a limited number of available qubits.

The above transformations lead to the Hamiltonian

\[ H = \sum_{k=-L/2+1}^{L/2} \left[ \lambda - \cos \left( \frac{2\pi k}{L} \right) \right] \hat{c}_k^\dagger \hat{c}_k + i \sin \left( \frac{2\pi k}{L} \right) \left( \hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \hat{c}_{-k} \hat{c}_k \right), \quad (A10) \]

Finally, in order to diagonalize the Hamiltonian, we have to apply a Bogoliubov transformation:

\[ a_k = u_k \hat{c}_k + iv_k \hat{c}_k^\dagger, \]
\[ a_k^\dagger = u_k \hat{c}_k^\dagger - iv_k \hat{c}_k. \quad (A11) \]

This transformation can be achieved with gates (red gate in Fig. 7) of the form

\[ B_k = \begin{pmatrix} \cos \frac{\theta_k}{2} & 0 & i \sin \frac{\theta_k}{2} \\ 0 & 1 & 0 \\ i \sin \frac{\theta_k}{2} & 0 & i \cos \frac{\theta_k}{2} \end{pmatrix}. \quad (A12) \]
Figure 9. Classically computed operator entanglement entropy of the circuits as a function of the number of blocks and the nonequilibrium protocol, for $L = 4$ (blue) and $L = 8$ (orange) qubits. The dashed horizontal lines indicate the Page values $S_{\text{Page}} = L \ln 2 - 1/2$, the vertical lines indicate the value for $L - 1$ blocks chosen for our simulations, see also Fig. 2. $L - 1$ blocks are sufficient to generate entanglement close to the Page value.

Simulation prepares the correct thermal ensemble for different inverse temperatures $\beta$ and the entire range of initial energies. Note that we observe a slight temperature dependence in the fluctuations: Low energy states are prepared more often than predicted by theory; higher energy states are slightly underrepresented. As we discussed in Sec. VI, the measurement itself is a dissipative process, causing decay from the excited to the ground state of the qubits.

In the case of $L = 4$ qubits, we obtain the density matrix $\rho_{\text{sim}}$ of the state created in part (B) of Fig. 2 using quantum state tomography [59] and compare it with the noiseless simulation $\rho_{\text{ideal}}$. We obtain a many-particle fidelity $F = \frac{1}{n} \text{tr} \rho_{\text{sim}} F_{\text{ideal}}^\dagger \rho_{\text{ideal}}^\dagger \approx 0.59$. As before we apply no error mitigation in this case.

### Appendix B: Analysis of the nonequilibrium protocols

This section is dedicated to an analysis of the specific circuit protocols we selected to use in this study. We show here numerically that we are operating in a nontrivial quantum many-body regime, by computing the operator entanglement entropy of our circuits [60] and the work distribution. Finally, we present results for different choices of the one-body random unitary gates and show that the specific choice of the random gates has only a minor impact on the accuracy for validation of Eq. (1).

1. **Operator entanglement entropy**

We analyze our circuits from an entanglement perspective and show that our ideal circuits are sufficient to create entanglement close to the Page value.

For a given system, we can choose complete basis sets of operators $\{A_i\}$ and $\{B_j\}$ which are orthonormal and have only support on the subsystem $A$ and $B$ respectively. An operator $O$ can now be decomposed as

$$O = \sum_{i,j} O_{i,j} A_i \otimes B_j.$$  

(B1)

This allows the notion of a reduced operator density matrix $\rho_{\text{op}}$ with matrix elements

$$\left( \rho_{\text{op}} \right)_{i,j} = \sum_k O_{i,k} O_{j,k}^\dagger.$$

(B2)

The operator entanglement entropy is given by

$$S = - \text{tr} \left( \rho_{\text{op}} \ln \rho_{\text{op}} \right).$$

(B3)

with the partition into two subsystems across the central bond.

We can compute the operator entanglement entropy of the unitary operator of our protocol using a partition across the central bond of the system. The results are shown in Fig. 9. It is obvious that our chosen operators with $L - 1$ blocks already show an entropy close to the Page-value [54] $S_{\text{Page}} = L \ln 2 - 1/2$.

2. **Work distribution**

The work distributions for two different inverse temperatures $\beta = 0.1$ and $\beta = 1.0$ are shown in Fig. 10. We obtain a roughly Gaussian distribution for both temperatures. There are also no additional long tails in the distribution, which is beneficial for the number of required measurements to test the Jarzynski equality [49].

At this point it is also interesting to compare the work distribution with the free energy difference. The free energy difference is marked in Fig. 10 by a dashed black line, the average work by a dashed magenta line. It holds $\Delta F < \langle W \rangle$ and thus the second law of thermodynamics holds, as expected. However, it is also visible that with a finite probability the extracted work is larger than the free energy difference.

Furthermore, in order to test that we are not in an adiabatic regime we compute $\langle \beta W_{\text{diss}} \rangle$ and comparing it to Eq. (1), as is done in Table III.

Since $W_{\text{diss}} \gg 0$, it follows that the adiabatic approximation does not hold for our chosen protocols.

3. **Different circuit realizations**

Finally, we check the effect of different single-qubit random unitaries on the output of our results. To do so, we repeat our

| $\beta$ | $\ln \langle e^{-\beta W_{\text{diss}}} \rangle$ | $\langle \beta W_{\text{diss}} \rangle$ |
|--------|---------------------------------|----------------|
| 0.1    | 0.01                            | 0.004          |
| 0.5    | 0.08                            | 0.27           |
| 1.0    | 0.23                            | 1.03           |

Table III. $\langle e^{-\beta W_{\text{diss}}} \rangle$ and $\beta W_{\text{diss}}$, experimental data for $L = 8$ qubits. The data indicate that our chosen protocol is in the non-adiabatic regime, where $\langle W_{\text{diss}} \rangle = 0$. 

FIG. 10. Histograms of the work distribution $P(W)$ for the protocol in Fig. 2 with seven blocks and $L = 8$ qubits: theory prediction (red) vs. experimental simulations (blue). The free energy difference $\Delta F$ is indicated by a dashed black line, the average work by a magenta line. Although the measured work can be smaller than the free energy for some shots, the average work is larger than the free energy difference and the second law of thermodynamics thus holds. The work distributions have a nearly Gaussian shape. The absence of strong tails in the work distribution reduces the number of required measurements.

The experiment for 4 qubits and 3 layers on ibm_perth for different circuit realizations, by choosing different random unitary gates. As we can see in Fig. 11, the deviation from Jarzynski’s equality does not depend strongly on the particular choice of random gates in our circuits.

**Appendix C: Statistical fluctuations**

The following section gives a quantitative analysis of the statistical uncertainties in the case of a finite number of measurements. For the scrambling circuits we choose in our simulations, we can use additional assumptions to get simple estimates for the size of the statistical fluctuations. This is especially helpful if we want to estimate the number of shots needed to estimate the free energy difference with a given accuracy.

To do so, consider the quantity

$$\Delta P = \left( e^{-\beta(W_{\text{diss }} - \Delta F)} \right).$$  \hspace{1cm} (C1)

This is just another representation of Jarzynski’s equality from Eq. 1. Given a perfect experimental realization including an infinite number of measurements, we expect $\Delta P = 1$. All deviations from this value can therefore be assigned to statistical errors, or errors coming from dissipative noise. Note that we consider $\Delta P$ instead of Eq. (1), since this representation is easier to handle analytically. Furthermore, in the limit of small deviations, the first order Taylor expansions around unity for $\Delta P$, and zero for Eq. (1), agree.

Given the eigenenergies of the initial and final Hamiltonians, the contribution $e^{-\beta \Delta F} = Z_f / Z_i$ can be computed exactly. Thus, any error originates from the measurement of the work distribution. We write

$$\left\langle e^{-\beta W} \right\rangle = \sum_{m,n} P_m K_{m\rightarrow n} e^{-\beta (E^m_f - E^n_i)}. \hspace{1cm} (C2)$$

Here $P_m$ denotes the probability to prepare a given initial eigenstate. In the optimal case of infinitely many measurements and error-free preparation $P_m = 1 / Z e^{-\beta E^m_i}$; $K_{m\rightarrow n}$ is the transition matrix of the process, defined in Sec. II.

There are two generic ways for errors to occur. The first one is as a statistical error in $P_m$,

$$P_m = \frac{1}{Z} e^{-\beta E^m_i} + \delta P_m. \hspace{1cm} (C3)$$

The first term on the right-hand-side is the probability distribution of the canonical ensemble. The second term denotes the error, with satisfies the sum rule $\sum_m \delta P_m = 0$. For a large enough number of states, we can assume the errors to be independent; then they are described by a binomial distribution, and scale as

$$\delta P_m \propto \sqrt{\frac{e^{-\beta E^m_i}}{Z_i} \left( 1 - \frac{e^{-\beta E^m_i}}{Z_i} \right)^{-1/s}}, \hspace{1cm} (C4)$$

where $s$ denotes the number of shots. This expression is the variance of a binomial distribution for an event occurring with probability $e^{-\beta E^m_i} / Z_i$.

The second way an error can occur, is through a measurement of $K_{m\rightarrow n}$. We can write

$$K_{m\rightarrow n} = \tilde{K}_{m\rightarrow n} + \delta K_{m\rightarrow n}, \hspace{1cm} (C5)$$

where $\tilde{K}_{m\rightarrow n}$ comprises any unitary or doubly-stochastic contributions that Jarzynski’s equality is insensitive to. Using the (simplifying) assumption that the correct size of each matrix element is roughly $1/D$ with $D = 2^L$ (this is justified by
is the sum of the variances), we find that the second term, and invoking the central limit theorem (the variance of a sum which should not prefer any particular eigenstate transitions), Equation (C7) is Jarzynski’s equality. Assuming that all terms $K_{m,n}$ scales as

$$\delta K_{m,n} \propto \sqrt{\frac{Z_i}{D s e^{-\beta E_m^i}}}. \quad (C6)$$

This is again the standard deviation for a binomial process of an event with probability $1/D$ and an effective number of repetitions $s e^{-\beta E_m^i}/Z_i$. We used here $(1 - 1/D) \approx 1$.

Taking these considerations into account, we can now divide the contributions of the fluctuations into four parts:

$$\Delta P = 1 \quad (C7)$$

$$+ \frac{Z_i}{Z_f} \sum_{m,n} \delta P_m \delta K_{m,n} e^{-\beta (E_m^i - E_n^i)} \quad (C8)$$

$$+ \frac{1}{Z_f} \sum_{m,n} \delta K_{m,n} e^{-\beta E_n^i} \quad (C9)$$

$$+ \frac{Z_i}{Z_f} \sum_{m,n} \delta P_m \delta K_{m,n} e^{-\beta (E_m^i - E_n^i)} \quad (C10)$$

Equation (C7) is Jarzynski’s equality. Assuming that all terms $K_{m,n} \sim 1/N$ (as a consequence of using random circuits, which should not prefer any particular eigenstate transitions), and invoking the central limit theorem (the variance of a sum is the sum of the variances), we find that the second term, Eq. (C8), scales as

$$\frac{Z_i}{D \sqrt{s}} \sum_{E_m} e^{\beta E_m^i} \left( 1 - \frac{e^{-\beta E_m^i}}{Z_i} \right). \quad (C11)$$

In turn, the third term is proportional to

$$\frac{Z_i}{D s} \sum_{E_m} e^{-\beta E_m^i} \sum_{E_n} \frac{e^{-2\beta E_n^i}}{Z_i^2}, \quad (C12)$$

and the last term is of order

$$\frac{Z_i}{\sqrt{N s Z_i}} \sum_{E_m} e^{2\beta E_m^i} \left( 1 - \frac{e^{-\beta E_m^i}}{Z_i} \right) \sqrt{\sum_{E_n} e^{-2\beta E_n^i}}. \quad (C13)$$

Let us now test these expressions and the underlying assumptions we made above. Figure 12 shows the scaling of the errors for a noise-free quantum simulation (red) and a comparison with the exact error bars using the exact size of the matrix elements (blue). The data show that the simplification we used to compute error bars is well justified.

**Appendix D: Comparison with previous experiments**

In this appendix, we give the details of the comparison of our results to previous work, cf. Table II.

We use the definition from Eq. (17) to compare our simulation with previous experiments on systems with finite Hilbert space dimension. To do so, we extract the Hamiltonian, the inverse temperature $\beta$ and the measurement data for the validation of Eq. (1) from the simulations. Using these data, the evaluation of Eq. (17) is straightforward.

In the experiments [28, 30, 32, 33], the underlying Hamiltonian was either a spin-1/2 system or the transverse field Ising model for up to three qubits. We extracted the data for the validation from Fig. 3 of Ref. [33], from Fig. 3 of Ref. [28], from Fig. 3 of Ref. [30], Fig. 3 of Ref. [32] and Table 1 of [29]. The case of Ref. [31] is special: in their setup the authors chose $\beta = 0$, where Jarzynski’s equality is trivially obeyed, as can be directly seen from Eq. (1).

In the case of the trapped ion experiment [12], the model was a harmonic oscillator. In order to compute Eq. (17), we cut off after the lowest 10 modes, and normalized $\beta$ by the energy gap of the harmonic oscillator. For the extraction of the data, we considered Table 1 of [12], using the ramp time of 5 $\mu$s.

**Appendix E: Technical data of the various quantum devices**

The technical details, including coherence times, thermalization times, and gate times, as well as the average two-qubit fidelities on the different devices we used, are shown in Table IV.
Table IV. Technical data of the various quantum devices. $T_1$ is the relaxation rate of diagonal matrix elements in the density matrix, while $T_2$ denotes the relaxation rate of off-diagonal elements [58]. $T_\text{g}$ denotes the average execution time of the native two-qubit gate on each of these devices. The average two-qubit fidelity is the average fidelity of the system-specific two-qubit gate. While the qubit fidelity is comparable for all devices, $T_1$ varies over several orders of magnitude, depending on the underlying architecture.

| Device name        | # Qubits | $T_1[\mu s]$ | $T_2[\mu s]$ | $T_\text{g}[\mu s]$ | Average two-qubit fidelity |
|--------------------|----------|--------------|--------------|----------------------|---------------------------|
| ibm_perth [61]     | 7        | 134          | 146          | 0.44                 | 0.988                     |
| ibmq_guadalupe [61]| 16       | 106          | 119          | 0.4                  | 0.99                      |
| IonQ [56]          | 11       | $10^{10}$    | $2 \times 10^3$ | 200                  | 0.96                      |
| Rigetti Aspen-11 [62] | 40     | 30           | 14           | 0.18                 | ~0.93                     |
| quantumium.hqs-lt-s1 [63] | 20   | $>10^9$      | $3 \times 10^6$ | 28                   | 0.997                     |

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