Third law of thermodynamics and the scaling of quantum computers

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The third law of thermodynamics, also known as the Nernst unattainability principle, puts a fundamental bound on how close a system, whether classical or quantum, can be cooled to a temperature near to absolute zero. On the other hand, a fundamental assumption of quantum computing is to start each computation from a register of qubits initialized in a pure state, i.e., at zero temperature. These conflicting aspects, at the interface between quantum computing and thermodynamics, are often overlooked or, at best, addressed only at a single-qubit level. In this work, we argue how the existence of a small, but finite, effective temperature, which makes the initial state a mixed state, poses a real challenge to the fidelity constraints required for the scaling of quantum computers. Our theoretical results, carried out for a generic quantum circuit with N-qubit input states, are validated by experiments performed on a real quantum processor.

I. INTRODUCTION

Quantum computers represent the ultimate frontier in information processing, with the objective to obtain quantum advantage in solving computational problems that classical computers cannot address in any feasible amount of time [1, 2]. So far, one of the biggest obstacles to this endeavour has been noise, that is responsible for the decay of quantum coherence and correlations [3, 4] in quantum states, especially pure states which are notoriously hard to preserve. Their degradation hinders the exploitation of quantum resources such as quantum superposition and entanglement. This issue has led to the current paradigm known as Noisy Intermediate Scale Quantum (NISQ) regime [5], whereby one exploits quantum computers with a modest amount of noisy qubits. To obtain a quantum advantage, however, we will need to develop large-scale quantum computers with thousands of highly coherent qubits. Quantum error correction protocols [6, 7], assisted by the statements of the quantum threshold theorem [8, 9], can help in overcoming quantum state degradation. However, experiments on existing NISQ devices [10, 12] still lack the high-fidelity required for error correction. For this reason, the analysis of thermodynamical and energetic resources, has recently emerged in the literature as an useful tool to study the fundamental limits of quantum computation, with several implications on quantum gates [13, 14], quantum annealers [15, 16] and quantum error-correction [17].

In the following, we will focus on thermodynamic limits for quantum state preparation, and on their consequences in obtaining high fidelity in multi-qubit quantum registers. The very existence of pure states and the limits to their preparation have to face Nernst’s unattainability principle, also known as the third law of thermodynamics [18], stating that cooling a physical system to the ground state ideally requires infinite resources. Since pure states can be brought to the ground state (and vice-versa) by means of finite-cost transformations, i.e., unitary operations, in order to abide to the third law, the preparation of pure states necessarily involves an infinite resource cost. This issue has been recently brought to light in the quantum thermodynamics community with implications to quantum measurement [19], purification [20] and cooling [21]. The simplest and most fundamental case of state preparation is the initialization of a qubits register to the computational state |00...0⟩ by means of the operation denoted as reset. Single-qubit reset, has been investigated in numerous platforms, some of which are: solid state, such as silicon [22] or rare-earth ion-doped crystals, both in spin ensembles [23, 24] and single ions [25], NV centers in diamond [26], superconducting qubits [27, 30], microwave photons [31, 32] and trapped ions [33, 35]. However, |00...0⟩ being a pure state, it is subject to the thermodynamic constraint originated by the Nernst’s principle.

In this work, we will go beyond the thermodynamics of the single-qubit reset, showing that in real-world quantum computers there exist a thermodynamic limit to the initialization of multi-qubit registers that, other than being a fundamental theoretical topic, has practical implications on the scaling of quantum computers. In fact, although the reset (or initialization) of single-qubits has been proven to be realized with high-fidelity (even above 99.9%) [36], we are going to analytically prove and experimentally verify that even a small initialization error on a multi-qubit register may dramatically reduce the fidelity of a multi-qubit states by following a scaling law that directly stems from Nernst’s principle. We argue that, in order to go beyond NISQ devices, substantial efforts are needed to improve not only the fidelity of single gates, but also the quality of initialization of multi-qubit registers. Thus, with this work, our aim is to help improving the design of quantum protocols and devices that
properly takes into account fundamental thermodynamic constraints, hitherto neglected.

II. FIDELITY SCALING

The usual assumption in quantum computation is to initialize the qubits register in the computational state $|00...0\rangle$. Here, we want to investigate how the fidelity of a quantum computer is affected by an imperfect preparation of the initial $|00...0\rangle$ register. Using the formalism of density matrices, the initial $N$-qubit pure state (target state) we wish to prepare is

$$\sigma_0 \equiv \bigotimes_{i=1}^{N} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

that, by definition, is a zero temperature state. However, from the Nernst’s unattainability principle we are bound to prepare states that have an arbitrary small, but finite, temperature. We assume thus that the real initial state of the system is the thermal state $\rho_0 = e^{-\beta H}/Z$ (where $Z$ is the appropriate partition function) that reads explicitly:

$$\rho_0 \equiv \bigotimes_{i=1}^{N} \frac{1}{1 + e^{-\beta \Delta E}} \begin{pmatrix} e^{-\beta \Delta E} & 0 \\ 0 & 1 \end{pmatrix}$$

where $\beta$ is the effective inverse temperature of the initial (prepared) state and $\Delta E$ is the energy difference between the states $|0\rangle$ and $|1\rangle$. It is worth noting that the effective inverse temperature $\beta$ is not the actual inverse temperature of the environment in which our quantum computer is located (albeit it will depend on it), but is a parameter that takes into account on average all the sources of disturbance that prevent our system to be in a perfectly pure state. For this reason, we will refer to it as an effective temperature. In this regard, observe that our choice to take a global constant value for the effective inverse temperature $\beta$, instead of setting different inverse temperatures $\{\beta_1, ..., \beta_N\}$ for each qubit, stems from considering the average error on the state initialization of the target state $\sigma_0$ on all the $N$ considered qubits for sake of clarity. Thus, without loss of generality, we can consider an average effective temperature that, in turn, makes our model easier to interpret. Moreover, let us also note that with this notation, in the limit of zero temperature ($\beta \to \infty$), the $\sigma_0$ state is recovered, while in the opposite limit of infinite temperature ($\beta \to 0$) one gets the maximally mixed state $I_{N \times N}/2^N$. We also recall that, given two density matrices $\rho$ and $\sigma$, representing the states of a quantum system, the fidelity between them is usually defined as $F(\rho, \sigma) = \sqrt{\text{Tr} \left[ \sqrt{\rho} \sigma \sqrt{\rho} \right]}$ [37].

Now, after setting our notation and initial assumptions, we formally show how the fundamental limit imposed by Nernst’s principle to the quantum state initialization affects the scaling of quantum computers. In doing this, let us initially take a perfect (in the sense of noiseless) unitary transformation $U$ operating on an ensemble of $N$ qubits, such that $\rho_1 \equiv U \rho_0 U^\dagger$ and $\sigma_1 \equiv U \sigma_0 U^\dagger$ are the resulting density operators after the application of the transformation. Then, we can find the analytical expression for the fidelity $F(\rho_1, \sigma_1)$ as a function of the parameters $N$ and $\beta$. Since the fidelity is invariant under any unitary transformations and $\sigma_0$ is a pointer state, we can prove that

$$F(\rho_1, \sigma_1) = F(\rho_0, \sigma_0) = \text{Tr} [\rho_0 \sigma_0] \quad (3)$$

By substituting the explicit form of $\rho_0$ and $\sigma_0$ in Eq. (3), we obtain the following result for the scaling of $F(\rho_1, \sigma_1)$ as a function of the parameters $N$ and $\beta$:

$$F(\rho_0, \sigma_0) = (1 + e^{-\beta \Delta E})^{-N} \quad (4)$$

that is valid independently on which unitary transformation $U$ is applied. Eq. (4) clearly shows that, even having at disposal any perfect unitary transformations $U$, a value slightly bigger than zero for the initial inverse temperature $\beta$ of the real state $\rho_0$ can end up hindering the scaling (i.e., $N \to \infty$) of the considered quantum circuit or algorithm. The reason behind this result being so general, lies again in the thermodynamic considerations behind the Nernst’s unattainability principle, and thus in the divergent cost of attaining a perfect pure state (i.e., with $\beta \to \infty$). In fact, it now becomes clear, that the issue of scaling quantum computers regards two competing limits:

$$\lim_{N \to \infty} \lim_{\beta \to \infty} F(\rho_0, \sigma_0) = 1 \quad (5)$$

$$\lim_{\beta \to \infty} \lim_{N \to \infty} F(\rho_0, \sigma_0) = 0 \quad (6)$$

Eq. (5) states simply that if one is able to initialize a qubit in a pure quantum state, then in principle a perfect, arbitrarily large quantum register can be realized. While, Eq. (6) reflects the evidence that, for finite temperature, increasing the size of the quantum device necessarily entails a decrease in the attainable initial state fidelity $F(\rho_0, \sigma_0)$ that will eventually disrupt the computation. The non-commuting nature of the two series of limits (5) and (6) is the second result of this work. In addition, the results of Eq. (5) and Eq. (6) remain valid even if the real initial state $\rho_0$ contains residual quantum coherence (in the form of off-diagonal terms) originated by non-ideal state initialization routines. Refer to the Supplemental Material for the proof of such result. Accordingly, in order to move beyond NISQ devices, we need to prepare pure states with increasing fidelity by properly taking into account also the needed resources, at least at the energetic level. In doing this, quantum state initialization could need to be improved at a faster rate than the one at which the size of quantum computers increases.

Let us now analyze the more general case in which a noisy quantum circuit (or, in general, a quantum channel) is applied to $\rho_0$. In case the quantum channel is responsible for non-unitary dynamics, the value $(1 + e^{-\beta \Delta E})^{-N}$ remains, for most non-unitary maps, an
upper bound to the attainable fidelity $\mathcal{F}(\rho_1, \sigma_1)$ of the final computation. However, there are some cases in which this does not hold and the application of a noisy quantum channel actually improves the initial fidelity. This can be pictured by considering the extreme case whereby $\rho_0$ is the identity state on the $2^N$ dimensional Bloch sphere. This state is the fixed point of the unitary dynamics, so one could easily find non-unitary maps that kick the system out of the identity state, thus improving the final fidelity with respect to the initial one. Other than the identity state, there will also be a volume of states around the identity for which this reasoning is valid and the initial fidelity $\mathcal{F}(\rho_0, \sigma_0)$ is no longer an upper bound to $\mathcal{F}(\rho_1, \sigma_1)$. The theory behind these concepts is discussed in the Supplemental Material. However, for the specific case of depolarizing quantum channels, which are commonly used to model noisy quantum computers [33, 34], it can be proved that (see the Supplemental Material for the proof):

$$\mathcal{F}(\rho_1, \sigma_1) \leq \mathcal{F}(\rho_0, \sigma_0) = \left(1 + e^{-\beta\Delta E}\right)^{-N}. \quad (7)$$

Overall, these findings are quite general and hold – regardless of coherent and possible non-unitary sources of noise – as an upper bound to the attainable fidelity of a generic operation $U \in \text{SU}(2^N)$, given the constraints imposed by thermodynamics.

To better understand our results, we provide a quantitative gauge of the attainable precision (in terms of the fidelity function) of quantum computing, given a nonzero temperature of the initial qubit states. In this regard, in Fig. 1 one can observe a plot of the fidelity $\mathcal{F}(\rho_0, \sigma_0)$ with respect of the size $N$ of the qubit register for some values of single qubit error rates $\eta_i$ related to the effective temperature $\beta$ by means of the relation $\eta = 1 - (1 + e^{-\beta\Delta E})^{-1}$. In Fig. 1 it is apparent a sharp decay of the fidelity $\mathcal{F}(\rho_0, \sigma_0)$ while increasing the number $N$ of qubits; even by starting with quite accurate single qubit initialization, the fidelity will eventually start degrading.

Once realized that perfect initialization may be challenging due to strict thermodynamic constraints imposed by the third law of thermodynamics, one shall necessarily perform quantum state initialization with an error good enough to ensure that the fidelity $\mathcal{F}(\rho_0, \sigma_0)$ – as provided by Eqs. (3) and (4) – is equal to the target value required to the operation. To put this into perspective, to have a target fidelity of 90% for a quantum computer of 1000 qubits, the error on the single qubit initialization has to be well below $10^{-4}$ that, to our knowledge, is the best recorded value [33, 34].

A similar kind of scaling, was already observed for the preparation of GHZ states, both theoretically [11] and experimentally [12] (in particular, we refer to Fig. 17b) on a 24-qubits trapped ion platform. However, GHZ states are highly nontrivial, with respect to the $|00...0\rangle$ register state, thus requiring the implementation of a Mølmer-Sørenson gate. In such a case, the dominant effect explaining the fidelity decay is likely due to the number of operations (scaling as $\sim N^2$) required to prepare the GHZ state. Of course, the simpler case (analyzed in this work) concerning the preparation of the factorized state $|00...0\rangle$ on $N$ qubits, as proved above, always remains valid as an upper bound for the attainable fidelity. As an example, we estimate that for the values of $\eta \sim 5 \times 10^{-3}$ reported in [12], the fidelity to initialize the $|00...0\rangle$ state for the 24-qubits will be $\sim 90\%$, while the actual measured fidelity after the circuit required to create the GHZ state is $\sim 50\%$.

### III. Experiments

In this section, we test experimentally our theoretical findings, with the aim to understand in quantitative terms how the fidelity of current flagship quantum device scales as a function of the system’s size and in relation to the quantum state initialization. For this purpose, experiments are performed using a superconducting quantum computer provided by IBM [10]. Specifically, our experiments are run on the ibm-lagos quantum computer that, with 7 qubits and a quantum volume [33] of 32, was the larger device at our disposal.

The first realized scaling experiment consists in locally measuring the initial register state $|0\rangle^\otimes N \equiv |00...0\rangle$ immediately after its preparation. For each value of $N$, the experiment is repeated 5000 times to collect statistics. Note that in such a case the fidelity $\mathcal{F}(\rho_0, \sigma_0)$ is equal to the frequency by which the $|0\rangle^\otimes N$ state is measured. By then performing the experiment for different qubits’ number $N$, we obtain the results reported in Fig. 2. From the figure one can observe that, while...
the single-qubit initialization fidelity is almost 99%, as the qubit count increases this value drops significantly to around 92%. To quantitatively evaluate the fidelity scaling, we assume the fidelity to be scaling as Eq. (4), and we fit the value of $\beta \Delta E$ over the experimental data, getting a value of $\beta \Delta E = 4.35 \pm 0.03$ with a coefficient of determination $R^2 = 0.976$. The resulting curve, whose analytical expression is provided by Eq. (4), is plotted as the dashed line in Fig. 2. Since IBM provides us with the values of $\Delta E$ [10] for each qubit of our processor (all around 5 GHz), we can thus compute the value of the effective temperature $\beta$, that for the realized experiments is placed at 56.80 ± 1.21 mK. This effective temperature, as expected, is a bit higher than the physical temperature of the fridge ($\sim$ 15 mK), since it takes into account also the effect of other sources of noise such as measurement-induced errors or single-gate errors. Note that our choice to take a global constant for the effective temperature gives a small discrepancy between the experimentally measured values and the theoretical scaling curve where, in the experiment, every qubit has its own effective temperature which is slightly different from the average one. The trend of the fidelity scaling provided by Eq. (4), with respect to the size $N$, is shown in the inset of Fig. 2 where the predicted fidelity is evaluated for a circuit composed by a larger number of qubits. We remark here that, since the number of qubits at our disposal was just up to $N = 7$, this scaling is an extrapolation from our theory and the fit we provide does not constitute a proof that the scaling we propose is indeed the correct one.

Hence, from the results in Fig. 2, it becomes evident the so fundamental role played by quantum state initialization for the effective realization of a large-scale quantum computer (or more generally a quantum device), before its fidelity dramatically decreases.

IV. RESET PROTOCOLS

We then focus on understanding how these results can be improved. The simplest way to reset a qubit is to wait for the relaxation time $T_1$ such that the environment acts as a reset for the qubit. Nevertheless, when $T_1$ is large (the meaning of “large” will depend on the application), such a reset procedure is not viable, as it will drastically increase the information processing time, i.e., the time interval to run the whole protocol all times needed for the desired goal. Therefore, active reset methods have been devised, which fall into two categories: conditional [44–46] and unconditional [30, 47, 48] resets. We employed a mixture of conditional resets methods and thermalization inspired by experiments performed by IBM [19] where we take a register of qubits, initially prepared in the superposition state $|+\rangle^{\otimes N} = (H |0\rangle)^{\otimes N}$ (with $H$ being the Hadamard gate) [20] is reset to $|0\rangle^{\otimes N}$ by means of $K$ consecutive conditional resets. In this conditional reset protocol, each qubit of the register is measured and then a NOT-gate is applied conditionally on the measurement outcome. Ideally, the register is reset to $|0\rangle^{\otimes N}$ with zero error, but practically its state is set to the density operator $\rho_K$.

In Fig. 3, the results of the conditional reset experiments, carried out on the IBM quantum computer ibm-lagos 7-qubits, are plotted for a varying number of resets $K$. As one can observe, by increasing the number of resets (i.e., employing more energy to carry out the reset protocol), the state reset fidelity increases up to a certain plateau, whose value depends on (i) the measurement readout error, (ii) the gate noise affecting the NOT operation, as well as (iii) the thermalization of the qubit due to the environment. We also observe that we can further increase the fidelity of our reset protocol by inserting a delay of 500$\mu s$ between two consecutive reset (dash-dotted lines in Fig. 3) during which the qubits thermalize with the environment. This delay value of 500$\mu s$ is the maximum that we could implement on our machine and we observed that, for different values, increasing the delay would lead to a better reset fidelity. A similar behaviour was also observed in [21] for a range of different processors. Let us also note that the difference between the results provided by the reset protocol applied both to a single-qubit register and to the 7-qubits register lies in the plateau’s value (that decreases as the size of the register increases) and not in the number $K$ of resets needed to reach the maximum allowed fidelity. Our findings are the hint that achieving greater fidelity values in state initialization protocols just for a larger amount of thermodynamic resources (i.e., energy and time) than
FIG. 3. Experimental fidelity between the quantum computational state $\sigma_0$ and the density operator $\rho_K$, solution of the conditional reset protocol, as a function of $K$. The latter denotes the number of consecutive conditional resets we performed. The circle markers are the fidelity values in applying conditional resets on a single-qubit register, while the cross markers identify the conditional resets on the 7-qubits register. Dashed lines refer to consecutive resets without delay and dash-dotted lines to resets with a delay of 500µs between them. The error bars are smaller than the size of the markers. We can observe that repeating more times the reset protocol (i.e., using more resources) improves the fidelity of the state initialization. However, after a certain number of repetitions, this improvement saturates due to the measurement errors that affect the conditional reset protocol.

the nominal case, as we quantified in Fig. 3

V. CONCLUSIONS

In conclusion, the resolution of any quantum state initialization protocol, as the ones addressed here, is constrained by the statement of the third law of thermodynamics, whereby the purification of a quantum state (equivalent to a cooling process in case of qubits) requires an increasing amount of resources (in terms of energy, time or space) as the desired purity value is higher.

Here, we have also proved, both theoretically and experimentally, that the larger the size of the quantum register we need to prepare, as well as of the quantum circuit we need to realize, the more expensive the initialisation protocol has to be. The observed scaling clearly follows the thermal distribution expressed by Eq. [5] for every finite value of the effective inverse temperature $\beta$ of the initial qubits register. We argue that this thermodynamic bound has to be carefully taken into account, not only from a purely theoretical point of view, but also from a technological one as we aimed to show with our experimental results. The solution to the challenge posed by this constraint, is to use better protocols and using more resources in order to reach the target fidelity values needed by the desired size of the register.

In this regard, it would be of great interest to compare different implementations of conditional and unconditional resets, as well as more recent ideas which avoid resets entirely [55]. A detailed study of all the variants of qubit reset is timely and of great importance to the future of quantum computing. In future investigations, it might also be interesting to explore if quantum computing can be redesigned, thus pushing efforts for a quantum computation operating (even partially) on mixed quantum states [53]. To conclude, we would like to stress the fundamental importance that the thermodynamical study of quantum systems will have for the development of quantum devices and the successful realization of large-scale quantum computers. As we showed in this work, considerations about energy dissipation, finite-temperature states and other thermodynamical quantities will be of fundamental importance for the next developments in practical applications of quantum computing.

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quantifies how much the channel is non-unitary. Our target state \( \sigma_1 \), on the other hand, would be \( \sigma_1 = U \sigma_0 U^\dagger \). Then, we check whether

\[
\mathcal{F}(\rho_0, \sigma_0) = \text{Tr}[\rho_0 \sigma_0] \geq \text{Tr}[\rho_1 \sigma_1] = \mathcal{F}(\rho_1, \sigma_1). \tag{15}
\]

For this purpose, \( \text{Tr}[\rho_1 \sigma_1] \) can be explicitly expressed as \( \text{Tr}[\rho_1 \sigma_1] = (1 - \lambda) \text{Tr}[\rho_0 \sigma_0] + \frac{\lambda}{2^N} \) by using the cyclic property of the trace. In this way, one obtains the following inequality:

\[
\text{Tr}[\rho_0 \sigma_0] \geq (1 - \lambda) \text{Tr}[\rho_0 \sigma_0] + \frac{\lambda}{2^N}. \tag{16}
\]

With some simple manipulations, the inequality (16) simplifies as

\[
\text{Tr}[\rho_0 \sigma_0] \geq 2^{-N}. \tag{17}
\]

Finally, by recalling the explicit expression of \( \text{Tr}[\rho_0 \sigma_0] \), we have that

\[
(1 + e^{-\beta \Delta E})^{-N} \geq 2^{-N} \tag{18}
\]

that is always true \( \forall \beta \geq 0 \). We have thus proved Eq. (7).

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**FIDELITY SCALING WITH GENERIC NON-UNITARY CHANNELS**

Here, we prove the conditions that allow for the validity of the bound in Eq. (7) for a generic non-unitary channel \( \Phi \), with \( \rho_1 = \Phi(\rho_0) \). For calculation purposes, we simply assume that the target transformation is the identity channel such that \( \sigma_1 = \sigma_0 \). Under these assumptions, the expression that we want to check, i.e.,

\[
\mathcal{F}(\rho_1, \sigma_1) \leq \mathcal{F}(\rho_0, \sigma_0), \tag{19}
\]

becomes the following inequality:

\[
\text{Tr}[\rho_1 \sigma_0] \leq \text{Tr}[\rho_0 \sigma_0]. \tag{20}
\]

From Eq. (20), by making explicit each terms in the inequality, one gets that

\[
\langle N | \Phi(\rho_0) | N \rangle \leq (1 + e^{-\beta \Delta E})^{-N}, \tag{21}
\]

i.e.,

\[
e^{-\beta \Delta E} \leq (\langle N | \Phi(\rho_0) | N \rangle)^{-1/N} - 1. \tag{22}
\]

Therefore, in order to satisfy the inequality (19), one has to require that

\[
\beta \geq -\frac{1}{\Delta E} \log \left( (\langle N | \Phi(\rho_0) | N \rangle)^{-1/N} - 1 \right). \tag{23}
\]

Eq. (23) depends on the specific map \( \Phi(\cdot) \) one is considering, and both sides of the inequality is dependent on \( \beta \): the left-hand-side explicitly, while the right-hand-side implicitly. Thus, the validity of Eq. (23) can be tested only once \( \rho_0, \Phi \) and \( N \) have been assigned. In general, there will be some particular quantum states and non-unitary quantum maps for which Eq. (19) is not satisfied, since counter-intuitively the application of a noisy channel may result in an increased value of the fidelity \( \mathcal{F} \). To better frame the meaning of inequality (23), let us look at a pathological case that does not satisfy Eq. (23), i.e., considering \( \beta = 0 \) that corresponds to take \( \rho_0 \) equal to the completely mixed state. Being such a state the fixed point of any unitary dynamics, there is no way to bring the real initial state \( \rho_0 \) closer to the target state \( \sigma_0 \) by means of a unitary operation. Hence, for the case of \( \beta = 0 \), the bound (23) is not verified, since there might exist at least one non-unitary channel/transformation (a quantum purification process in the considered pathological case) able to correctly modify the real initial quantum state and make it overlap with \( \sigma_0 \), such that the fidelity \( \mathcal{F}(\rho_1, \sigma_1) \) results increased. Accordingly, we can conclude that, while Eq. (19) holds for most quantum states and non-unitary maps, it may be violated, as proved by the pathological case with \( \beta = 0 \).