Thermalization in nature and on a quantum computer

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In this work, we put several questions related to the emergence of Gibbs states in quantum physics to rest. We show how Gibbs or thermal states appear dynamically in closed quantum many-body systems, by completing the program of dynamical typicality and by introducing a novel general perturbation theorem that is robust under the thermodynamic limit, rigorously capturing the intuition of a meaningful weak coupling limit. We discuss the physics of thermal states occurring and identify the precise conditions under which this happens. Based on these results, we also present a fully general quantum algorithm for preparing Gibbs states on a quantum computer with a certified runtime, including full error estimates, complementing quantum Metropolis algorithms which are expected to be efficient but have no known runtime estimate.

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How do thermal quantum states – cornerstones of a description in canonical ensembles in quantum statistical physics – arise from the underlying theory of quantum physics? This question, a long tradition as it obviously has, is in many ways still surprisingly wide open. Indeed, much progress was made only quite recently [1–12]; this is motivated and triggered both by new mathematical [5–10, 12, 13] and numerical [14] techniques becoming available, as well as by new experiments with quantum many-body systems in non-equilibrium [15].

This work aims at finally bringing – with new technical results – this question to rest. We prove equilibration towards a Gibbs state, without any approximations, from the underlying microscopic theory of quantum mechanics. Our results complete, to a large extent, both the kinematic and the dynamic approach towards a justification of statistical mechanics. Finally, we use our new insights into the process of thermalization to design a quantum algorithm that prepares Gibbs states with certified precision and runtime.

The three ingredients that enter the standard textbook proof of the canonical ensemble in classical statistical physics are: (i) the *equal a priory probability postulate* (also known as microcanonical ensemble), and an equilibration postulate (such as the second law), (ii) the assumption of *weak coupling*, (iii) an assumption about the *density of states* of the bath, namely, that it grows faster than exponentially with the energy and that it can be locally well approximated by an exponential [16]. Here each of these steps is rigorously generalized to the *pure state quantum statistical mechanics* approach [1–9]. In particular (i) is replaced by a (dynamical) typicality argument that follows directly from quantum mechanics and (ii) is made precise by proving a novel perturbation theorem that has applications far beyond the scope of the present article.

Finally we present a *quantum algorithm preparing Gibbs states* with full error bounds and explicit runtime bounds, invoking a new variant of phase estimation. Our algorithm nicely complements another algorithm with certified runtime that was recently proposed in [18] and recent developments on quantum Metropolis algorithms [12], which are expected to be efficient, but for which, unlike in our approach, no rigorous runtime estimates exist. A significant step towards constructing a certified (and in some cases efficient) algorithm was recently made in Ref. [17] (see Appendix F for a discussion).

Setting and notation. Throughout this work, we consider systems S weakly coupled to an environment B. Thus, the Hilbert space reads $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, where $\mathcal{H}_S$ and $\mathcal{H}_B$ (of finite dimensions d_S and d_B) are the Hilbert spaces of the subsystem and the "bath" respectively. The evolution of the total system is governed by the Hamiltonian $H = H_0 + V$, with eigenvalues and eigenvectors $\{E_k\}$ and $\{|E_k\rangle\}$ consisting of a uncoupled Hamiltonian $H_0 = H_S + H_B$, whose eigenvalues and eigenvectors we denote by $\{E_k^{(0)}\}$ and $\{|E_k^{(0)}\rangle\}$, and a coupling Hamiltonian V. In this setup, we rigorously clarify under which conditions under unitary time evolution $|\psi_t\rangle = \mathrm{e}^{-iHt}|\psi_0\rangle$ with $\psi_t = |\psi_t\rangle\langle\psi_t|$, the reduced state $\psi_t^S = \mathrm{Tr}_B\, \psi_t$ of the subsystem S does relax for most times to a Gibbs state $\rho^S_{\mathrm{Gibbs}} \propto \mathrm{e}^{-\beta H_S}$. By this we mean that for most times their trace distance $\mathcal{D}(\psi_t^S, \rho^S_{\mathrm{Gibbs}})$, which measures the physical distinguishability [22], is small. We assume that the Hamiltonians H and H_0 are non degenerate such that *time averaging* and *dephasing* in the eigenbasis give the same result

$$\omega = \overline{\psi_t} = \lim_{T\to\infty} \frac{1}{T}\int_0^T \psi_t \mathrm{d}t = \sum_k |E_k\rangle\langle E_k|\psi_0|E_k\rangle\langle E_k|. \tag{1}$$

If equilibration happens, then it happens towards the time averaged state [22], our insight into the mechanism of thermalization thus come from studying the reduced dephased state $\omega^S = \mathrm{Tr}_B\, \omega$.

"Natural thermalization": Conditions for Gibbs states to appear. In this section, by going through the points (i)-(iii), we prove the emergence of the canonical ensemble from quantum mechanics. The final conclusion is summarized in theorem 2. The central point of the argument is a novel perturbation theorem that relates spectral projectors of weakly interacting and non-interacting Hamiltonians in a physically relevant weak coupling limit. It allows us to connect results on dynamical equilibration and measure concentration with classical counting arguments and thereby prove a set of natural sufficient conditions for thermalization in quantum mechan-

ics.

A stepping stone in the following argument will be states that have a flat energy distribution in an interval $[E, E+\Delta]$, i.e., states that have the property that the diagonal elements in the energy eigenbasis in the subspace corresponding to the interval are all identical and all other diagonal entries vanish. We indicate such states, and their dephased states, by a subscript $\sqcap$ like in $\psi_\sqcap$ or $\omega_\sqcap$ and call them *rectangular states*. This class of states includes both *mixed states* (in particular the microcanonical state $\omega_\sqcap$) and *pure states*, and thus in general also initial states that can locally be far from equilibrium.

The equal a priory probability postulate (i) is replaced by a notion of (dynamical) typicality using results from Refs. [1, 2, 5]. In Ref. [1] powerful concentration of measure techniques are used to show that almost all states from a microcanonical subspace corresponding to a microcanonical energy window $[E, E+\Delta]$ locally look like the reduction of the corresponding microcanonical state, i.e., it is shown that for all but exponentially few of the states ψ from the subspace $\mathcal{D}(\psi^S, \omega_\sqcap^S)$ is small, where $\omega_\sqcap$ is the microcanonical state on the subspace. Refs. [5–7] complement this purely kinematic picture with a result concerning the dynamics of states that initially can even be far from equilibrium. Under one assumption on the spectrum of the Hamiltonian (non-degenerate energy gaps) it is shown that all reduced states on small subsystems of states with a high effective dimension tend to an equilibrium state and stay close to it for most times. Moreover all but exponentially few states from a microcanonical subspace have a high effective dimension.

The delicate issue, which has up to now not been addressed in the literature in a general and rigorous way, is the *weak coupling* approximation (ii) [6, 23]. The problem is, that due to the exponential growth of the Hilbert space dimension and the at most polynomial growth of the energy content, the spectrum of the non-interacting Hamiltonian H_0 becomes exponentially dense with increasing bath size. Which is why the *perturbative* limit, in which the coupling V is weak compared to the *gaps* of the non-interacting Hamiltonian H_0, in which it can be guaranteed that the energy eigenstates $|E_k\rangle$ of the full Hamiltonian $H = H_0 + V$ are close to product states $|E_k\rangle \approx |E_k^S\rangle \otimes |E_k^B\rangle$, is certainly *not the physically relevant weak coupling limit*. Even worse, in this limit memory effects provably prevent thermalization [9]. As in the classical setting, a coupling should be considered to be *weak* as long as it does not change the total energy in a *noticeable way*, which is equivalent to saying that the energy stored in the interaction is much less than our (microcanonical) uncertainty about the energy of the system, i.e., $\|V\|_\infty \ll \Delta$. This is the *relevant weak coupling limit* in which we prove equilibration towards a canonical state. We do this by relating the dephased/microcanonical state $\omega_\sqcap$ to the state $\omega_\sqcap^{(0)}$ dephased with respect to the non interacting Hamiltonian, for which we can then easily perform the partial trace.

Theorem 1 (interacting vs. non-interacting case)**.** *Let $\omega_\sqcap^{(0)}$ and $\omega_\sqcap$ be the dephased/microcanonical states belonging to the interval $[E, E+\Delta]$ with respect to H_0 and $H = H_0 + V$, then for every $\mathrm{gaps}(H_0) \ll \varepsilon < \Delta/2$ (the condition $\mathrm{gaps}(H_0) \ll \varepsilon$ contains a technicality made precise in the proof)*

$$\mathcal{D}(\omega_\sqcap^S, \omega_\sqcap^{S(0)}) \leq \mathcal{D}(\omega_\sqcap, \omega_\sqcap^{(0)}) \leq \frac{\|V\|_\infty}{\varepsilon} + \frac{\Delta\Omega + \Omega_\varepsilon}{2\,\Omega_{\min}} \quad (2)$$

where $\Omega_{\min}$ and $\Delta\Omega$ are the minimum, and the difference, of the dimensions of the support of $\omega_\sqcap^{(0)}$ and $\omega_\sqcap$, and Ω_ε is the total number of eigenstates of H and H_0 in the intervals $[E, E+\varepsilon]$ and $[E+\Delta-\varepsilon, E+\Delta]$.

The theorem shows that for any two initial (possibly pure) states that have a flat energy distribution in the interval $[E, E+\Delta]$ with respect to the Hamiltonians H_0 and H with $\|V\|_\infty \ll \Delta$ the distance of their reduced dephased states $\omega_\sqcap^{S(0)}$ and $\omega_\sqcap^S$ is small. In particular, assuming an approximately constant density of states, such that $\Omega_\varepsilon/(2\,\Omega_{\min}) \approx 2\varepsilon/\Delta$ and thus if $\Delta\Omega/\Omega_{\min} \approx 0$ the best choice for ε is $\varepsilon \approx (\|V\|_\infty \Delta/2)^{1/2}$ which gives

$$\mathcal{D}(\omega_\sqcap^S, \omega_\sqcap^{S(0)}) \lessapprox \frac{3\sqrt{2}}{2} \left(\frac{\|V\|_\infty}{\Delta}\right)^{1/2}. \quad (3)$$

We come back to the case of a non constant density of states in Appendix G after introducing the concept of temperature.

Proof. First note that by monotonicity of the trace distance and the triangle inequality

$$\mathcal{D}(\omega_\sqcap^S, \omega_\sqcap^{S(0)}) \leq \frac{1}{2}\|\omega_\sqcap - \omega_\sqcap^{(0)}\|_1 \leq \frac{\|E-F\|_1 + \Delta\Omega}{2\,\Omega_{\min}}, \quad (4)$$

where E and F are the projectors onto the support of $\omega_\sqcap$ and $\omega_\sqcap^{(0)}$ respectively and $\Omega_{\min/\max} = \min/\max(\mathrm{rank}(E), \mathrm{rank}(F))$ and $\Delta\Omega = \Omega_{\max} - \Omega_{\min}$. It remains to bound $\|E-F\|_1$. Let $\overline{E} = \mathbb{1} - E$ and $\overline{F} = \mathbb{1} - F$, then $E - F = E\overline{F} - \overline{E}F$ and thus $\|E-F\|_1 \leq \|E\overline{F}\|_1 + \|\overline{E}F\|_1$. To bound $\|E\overline{F}\|_1$ we decompose $E = E_i + E_e$ into an interior part E_i which is the projector onto the eigenstates from the interval $[E+\varepsilon, E+\Delta-\varepsilon]$ and the exterior part E_e and find $\|E\overline{F}\|_1 \leq \|E_i\overline{F}\|_1 + \|E_e\|_1$ (see Fig. 1). Using the inequality $\|\cdot\|_1 \leq \mathrm{rank}(\cdot)\|\cdot\|_\infty$, submultiplicativity of the rank, and that in all realistic situations we can ensure that $\mathrm{rank}(E_i) \leq \Omega_{\min}$ by choosing $\varepsilon \gg \mathrm{gaps}(H_0)$ not too small this can be recast into $\|E\overline{F}\|_1 \leq \Omega_{\min}\|E_i\overline{F}\|_\infty + \mathrm{rank}(E_e)$. Finally, from theorem V.II.3.1 in Ref. [19] it follows that $\|E_i\overline{F}\|_\infty \leq \|V\|_\infty/\varepsilon$. Repeating the argument for $\|\overline{E}F\|_1$, introducing the notation $\Omega_\varepsilon = \mathrm{rank}(E_e) + \mathrm{rank}(F_e)$, and putting everything together gives the desired result. □

The level counting argument (iii) – with is ultimately the reason for the exponential form $\rho^S_{\mathrm{Gibbs}} \propto \mathrm{e}^{-\beta H_S}$ – carries over to the quantum case in a straightforward way in the *absence* of coupling between system and bath [2, 6] and with a bit more work one can also obtain a rigorous general trace norm error bound. If the number of states of the

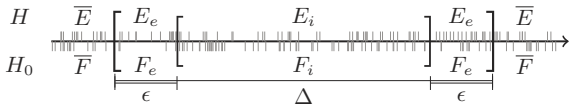

Figure 1. Definition of the projectors used in the proof of theorem 1.

bath $\Omega_\Delta^B(E^B)$ in the interval $[E^B, E^B + \Delta]$ is such that the proportion $\Omega_\Delta^B(E - E_k^S)/\sum_l \Omega_\Delta^B(E - E_k^S)$ is close to $\mathrm{e}^{-\beta E_k^S}/\sum_l \mathrm{e}^{-\beta E_l^S}$ for the given E and Δ and some β, then the distance of $\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S)$ is small. This can be guaranteed under a set of natural assumptions that are satisfied by a wide range of natural quantum many-body systems and that resemble the ones commonly used in classical statistical physics, such as continuous approximability and exponential increase of the density of states (Appendix A). In particular, for a bath consisting of m non-interacting spin-$1/2$ particles with a slightly varying on site field strength and average local energies of 0 and η one finds (Appendix B)

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S) \leq \frac{1}{2}(\mathrm{e}^{4\frac{\|H_S\|_\infty^2}{\eta^2 m}} - 1) + C \tag{5}$$

with C exponentially small in the bath size. We will use this bath later in our algorithm. For such a bath, the assumption of uniform density of states used in the derivation of Eq. (3) does not hold anymore. A discussion of theorem 1 for the exponential density of states is presented in Appendix G. In summary, Eq. (5), theorem 1, and the results on dynamical equilibration and random states from the unitary invariant measure derived in Ref. [1, 5] lead to the following conclusions:

Theorem 2. *(Kinematic) Almost all pure states ψ from a microcanonical subspace corresponding to an energy interval $[E, E+\Delta]$ of a weakly interacting, sufficiently large quantum system are locally close to a Gibbs state in the sense that for every* $\mathrm{gaps}(H_0) \ll \varepsilon < \Delta/2$ *the probability that*

$$\mathcal{D}(\psi^S, \omega_\sqcap^{S(0)}) \geq \frac{2d_S}{\sqrt{\Omega_{\min}}} + \frac{\|V\|_\infty}{\varepsilon} + \frac{\Delta\Omega + \Omega_\varepsilon}{2\,\Omega_{\min}} + \varepsilon' \tag{6}$$

drops of exponentially with $\Omega_{\min}\,\varepsilon'^2$. (Dynamic) Moreover, if the Hamiltonian in addition has non-degenerate energy gaps [5], all initial states $\psi_{\sqcap,0}$ with a flat energy distribution in the interval locally equilibrate towards ρ_{Gibbs}^S even if they are initially far from equilibrium in the sense that

$$\overline{\mathcal{D}(\psi_{\sqcap,t}, \omega_\sqcap^{S(0)})} \leq \frac{d_S}{2\sqrt{\Omega_{\min}}} + \frac{\|V\|_\infty}{\varepsilon} + \frac{\Delta\Omega + \Omega_\varepsilon}{2\,\Omega_{\min}}. \tag{7}$$

Both inequalities are robust against deviations from the rectangular distribution. If the bath has an exponentially increasing density of states basically only smoothness and a sharp cutoff towards higher energies is needed (for details see Appendix B).

"Artificial thermalization": A quantum algorithm for Gibbs state preparation. It follows from Eq. (5) and theorem 1 that all one has to do to prepare a Gibbs state is to prepare a state close to $\omega_\sqcap$ or $\omega_\sqcap^{(0)}$ on a suitable combination of system plus bath. This is what the quantum circuit shown in Fig. 2 does, without using any knowledge about the eigenstates of the Hamiltonian. It requires two registers. The first register R consists of r qubits initially in $|0\rangle$ and is used to perform quantum phase estimation. The second register Q holds quantum system plus bath and it is put into a rectangular state by performing the following steps:

1. *Initialization*. The register of the system is initialized into the completely mixed state [24], that is,

$$\rho_1 = \frac{1}{d}\sum_{k=1}^{d} |E_k\rangle\langle E_k| \otimes |0\rangle\langle 0|^r\,, \tag{8}$$

where d is the dimension of the total Hilbert space.

2. *Partial quantum phase estimation*. Second a new form of quantum phase estimation is performed, which comprises three steps: the application of r Hadamard gates on the qubits of the register, the application of controlled-U operations on the second register (with U raised to successive powers of two), and an inverse Fourier transform on the first register. After this operation, the state of the registers is,

$$\begin{aligned}\rho_2 &= U_{QPE}\left(\rho_1 \otimes |0\rangle\langle 0|^r\right) U_{QPE}^\dagger \\ &= \frac{1}{d}\sum_{s,s'=0}^{2^r-1}\sum_{k=1}^{d} \alpha_s(\varphi_k)\alpha_{s'}^*(\varphi_k)|E_k\rangle\langle E_k| \otimes |s\rangle\langle s'|\,,\end{aligned} \tag{9}$$

where $\varphi_k = E_k/\|H\|_\infty$ is the phase corresponding to $|E_k\rangle$ and $\alpha_s(E_k) = \frac{1}{2^r}\frac{1-\exp(2\pi\,\mathrm{i}(2^r\varphi_k - s))}{1-\exp(2\pi\,\mathrm{i}(\varphi_k - s/2^r))}$ is the amplitude of a probability distribution peaked around the value s that best approximates φ_k in binary format.

3. *Measurement*. Measuring the first q qubits of R, some value s_* is obtained and the system is left in the state

$$\rho_3 \propto \sum_{s,s'=s_*}^{s_*+\Delta_*}\sum_{k=1}^{d} \alpha_s(\varphi_k)\alpha_{s'}^*(\varphi_k)|E_k\rangle\langle E_k| \otimes |s\rangle\langle s'|\,, \tag{10}$$

where $\Delta_* = 2^{r-q}$ is the number of states of the ancilla register compatible with the measurement. By choosing r one can determine the width $\Delta = \|H\|_\infty 2^{-r}\Delta_*$ of the rectangular state that is prepared. The measured value of s_* determines the energy $E = \|H\|_\infty 2^{-q} s_*$ of the rectangular state, and thereby the temperature of the Gibbs state. To thermalize the subsystem at some particular temperature, the previous steps must be repeated until the desired energy is measured. This prevents us from preparing thermal states at very low temperatures since the probability $P(s_*)$ of getting outcome s_*,

$$P(s_*) = \sum_{k=1}^{d}\sum_{s=s_*}^{s_*+\Delta_*} |\alpha_s(\varphi_k)|^2 \simeq \frac{\Omega_\Delta(E)}{d}\,, \tag{11}$$

is proportional to the number of states $\Omega_\Delta(E)$ in the corresponding interval, which decreases exponentially with the inverse temperature β (see Appendix C). This is not a deficit of

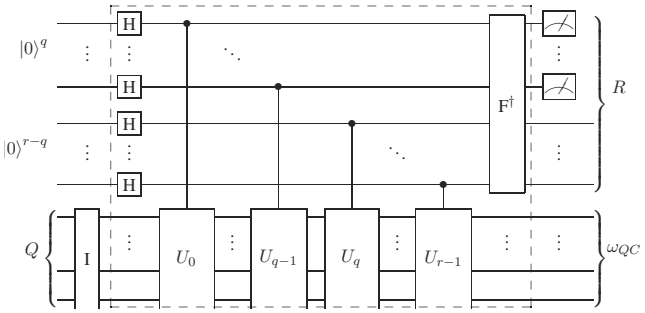

Figure 2. Quantum circuit that generates a dephased rectangular state $\omega_\sqcap^{(0)}$. I is the initialization gate, H are Hadamard gates, $U_\tau = U^{2^\tau}$, $U = \exp(-\,\mathrm{i}\,H_0/\|H_0\|_\infty)$ with $H_0 = H_S + H_B$, and $\mathrm{F}^\dagger$ is the inverse Fourier transform.

the algorithm, for otherwise QMA-hard problems could be efficiently solved. Any general algorithm will presumably have this feature [20]. The final state of Q is

$$\omega_{QC} = \mathrm{Tr}_R\, \rho_3 \propto \sum_{k=1}^{d} \left(\sum_{s=s_*}^{s_*+\Delta_*} |\alpha_s(\varphi_k)|^2 \right) |E_k\rangle\langle E_k| \,. \quad (12)$$

For large enough r, this state is close to the desired state $\omega_\sqcap$ with $E = \|H\|_\infty 2^{-q} s_*$ and $\Delta = \|H\|_\infty 2^{-r}\Delta_*$. The precise deviation ε of ω_{QC}^S from ρ_{Gibbs}^S,

$$\varepsilon = \mathcal{D}(\omega_{QC}^S, \rho_{\mathrm{Gibbs}}^S) \leq \mathcal{D}(\omega_{QC}, \omega_\sqcap^{(0)}) + \mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S). \quad (13)$$

depends on the density of states of system plus bath. A good candidate for the bath is the system of m non interacting spin-$1/2$ particles discussed before (Appendix B) and we give explicit results for the errors and the complexity of our algorithm for this bath:

Algorithm. *For any chosen $\lambda > 0$ and any given inverse temperature β and system Hamiltonian H_S, the algorithm presented in Fig. 2, using the bath with m spin-$1/2$ particles and energy scale $\eta = \sqrt{\lambda/m}\|H_S\|_\infty$ discussed before (Appendix B), prepares the system S of n qubits in a state within trace norm distance bounded by*

$$\varepsilon \leq 2^{q-r+2}\left(1 + \ln(2^{r-q})/\pi^2\right) \mathrm{e}^{\frac{2}{\lambda} + \beta\|H_S\|_\infty + \frac{\lambda\|H_S\|_\infty^2\beta^2}{8}} + \frac{1}{2}(\mathrm{e}^{\frac{4}{\lambda}} - 1) + C \quad (14)$$

with C exponentially small in m, to a Gibbs state ρ_{Gibbs}^S with a temperature in the interval $[\beta - \delta\beta, \beta + \delta\beta]$, where

$$\delta\beta \leq 2^{-q+2}\left(\frac{\lambda}{m}\right)^{1/2} \frac{1}{\|H_S\|_\infty}\left(1 + \frac{1}{\sqrt{m\lambda}}\right). \quad (15)$$

This is achieved using r ancilla qubits and running the algorithm an average number of

$$\overline{\sharp\ runs} \leq 2^q \left(\frac{\pi}{2m}\right)^{1/2} \mathrm{e}^{\frac{2}{\lambda} + \beta\|H_S\|_\infty + \frac{\lambda\|H_S\|_\infty^2\beta^2}{8}} \quad (16)$$

times, where each run requires the application of $n + 2r$ Hadamard gates, r controlled single qubit gates, $n + q$ with $q < r$ single qubit measurements and 2^r controlled unitary time evolutions under $H_0 = H_S + H_B$ for a time $1/\|H_0\|_\infty$.

Notice that, as the bath is a model of uncoupled spins, the time evolution under H_B can be implemented with m gates.

In practice, in absence of an oracle for the Hamiltonian of the system, the error produced to perform the U gate carries a second source of error that comes from the Trotter-Suzuki approximation. Nevertheless, this error can be suppressed at a polynomial cost for local Hamiltonians [18, 21].

The two contributions to the trace distance error ε (13) are computed in Appendices B and E, the average number of runs is computed in Appendix E and the error in the temperature comes from the discrete nature of energy measurement vie quantum phase estimation and is calculated in Appendix D. As is clear form Fig. 2, we need $\sum_{\tau=0}^{r-1} 2^\tau = 2^r$, U gates and the part of the circuit that does not correspond to the controlled time evolution, i.e., the initialization and the inverse Fourier transform, only requires the implementation of $n + m + 2r$ Hadamard gates, r controlled single qubit gates, and $n+m+q$ single qubit measurements.

Conclusions. Firstly, a set of sufficient conditions for thermalization in quantum mechanics has been presented. These conditions are basically a direct translation of the standard assumptions from classical statistical physics. Along the way, a perturbation argument for realistic weak coupling has been proven that we expect to have significant applications beyond the scope of this article. Secondly, a quantum algorithm for preparing thermal states has been presented. For a fixed large λ, the error of the algorithm can be made small by choosing an ancilla register of size $O(\beta^2\|H_S\|_\infty^2)$ for low temperatures. However, this does not contradict hardness results on problems like the local Hamiltonian problem due to the scaling of the runtime in $\beta\|H_S\|_\infty$. It constitutes an interesting perspective to fully flesh out the tightness of all involved bounds, and to engineer suitable baths that give rise to particularly efficient quantum algorithms.

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[1] S. Popescu, A. J. Short, and A. Winter, Nature Phys. **2**, 754 (2006).
[2] S. Goldstein, Phys. Rev. Lett. **96**, 050403 (2006); S. Goldstein, J. L. Lebowitz, C. Mastrodonato, R. Tumulka, and N. Zanghi, Phys. Rev. E **81**, 011109 (2010).
[3] H. Tasaki, Phys. Rev. Lett. **80**, 7 (1998).
[4] H. Dong, S. Yang, X. F. Liu, and C. P. Sun, Phys. Rev. A **76**, 044104 (2007).
[5] P. Reimann, Phys. Rev. Lett. **101**, 190403 (2008); N. Linden, S. Popescu, A. J. Short, and A. Winter, Phys. Rev. E **79**, 061103 (2009); A. J. Short, arXiv:1012.4622.

[6] P. Reimann, New J. Phys. 12, 055027 (2010).

[7] N. Linden, S. Popescu, A. J. Short, and A. Winter, New J. Phys. **12**, 055021 (2010); C. Gogolin, Phys. Rev. E **81**, 051127 (2010).

[8] O. Lychkovskiy, Phys. Rev. E **82**, 011123 (2010).

[9] C. Gogolin, M. P. Müller, and J. Eisert, Phys. Rev. Lett. **106**, 040401 (2011).

[10] M. Cramer, C. M. Dawson, J. Eisert, and T. J. Osborne, Phys. Rev. Lett. **100**, 030602 (2008); T. Barthel and U. Schollwöck, ibid. **100**, 100601 (2008).

[11] M.-H. Yung, D. Nagaj, J. D. Whitfield, and A. Aspuru-Guzik, Phys. Rev. A **82**, 060302(R) (2010).

[12] K. Temme, T. J. Osborne, K. G. Vollbrecht, D. Poulin and F. Verstraete, arXiv:0911.3635.

[13] M. P. Müller, D. Gross, and J. Eisert, Commun. Math. Phys., in press (2011).

[14] C. Kollath, A. Läuchli, and E. Altman, Phys. Rev. Lett. **98**, 180601 (2007); S. Manmana, S. Wessel, R. Noack, and A. Muramatsu, ibid. **98**, 210405 (2007); A. Flesch, M. Cramer, I. P. McCulloch, U. Schollwöck, and J. Eisert, Phys. Rev. A **78**, 033608 (2008); M. Rigol, Phys. Rev. Lett. **103**, 100403 (2009); M. C. Banuls, J. I. Cirac, and M. B. Hastings, arXiv:1007.3957.

[15] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature **415**, 39 (2002); L. E. Sadler, J. M. Higbie, S. R. Leslie, M. Vengalattore, and D. M. Stamper-Kurn, ibid. **443**, 312 (2006); S. Hofferberth, I. Lesanovsky, B. Fischer, T. Schumm, and J. Schmiedmayer, ibid. **449**, 324 (2007); S. Trotzky, Y.-A. Chen, A. Flesch, I. P. McCulloch, U. Schollwöck, J. Eisert, and I. Bloch, arXiv:1101.2659.

[16] L. D. Landau and E. M. Lifschitz, *Course of Theoretical Physics*, 3rd edition, Pergamon, Oxford (1980).

[17] E. Bilgin and S. Boixo, Phys. Rev. Lett. **105**, 170405 (2010).

[18] D. Poulin and P. Wocjan, Phys. Rev. Lett. **103**, 220502 (2009).

[19] R. Bhatia, *Matrix analysis* (Springer Verlag, New York, 1997).

[20] J. Kempe, A. Kitaev, and O. Regev, SIAM Journal of Computing, **35**, 1070 (2006).

[21] D. W. Berry, G. Ahokas, R. Cleve, and B. C. Sanders, Comm. Math. Phys. **270**, 359 (2007).

[22] See the introduction of Ref. [9].

[23] Ref. [2] only deals with the non interacting case. In Ref. [3] weak means that $\|V\|_\infty$ is much smaller than the level spacing of H_S, which is well defined in the limit of large baths, but still breaks down quickly even for relatively small subsystems and moreover the rigorous results are limited to cases where V only couples neighboring eigenstates. Ref. [4] contains a non rigorous discussion of the general case and numerical results suggesting that couplings much larger than the level spacing can be sufficiently weak for Gibbs states to emerge; a fact made rigorous in this work.

[24] One possibility is to prepare two registers maximally entangled between them. Another option is to use a single register and apply a Hadamard gate and a measurement on each qubit without looking at the outcome of the measurement. Notice that the advantage of this initial state is that it is the same for any Hamiltonian.

A Reduced density matrix of the dephased rectangular decoupled state – the general case

In this section, the distance between the subsystem of the dephased rectangular decoupled state and the Gibbs state $\mathcal{D}(\omega_\sqcap^{S(0)}, \rho^S_{\rm Gibbs})$ is computed. The discussion is similar to that in [6].

As all eigenvectors of H_0 are given by the tensor product of the eigenbasis of H_S and H_B, $|E_n\rangle = |E_k^S\rangle \otimes |E_q^B\rangle$, it is possible to trace the degrees of freedom of the bath of the decoupled rectangular state to get

$$\omega_\sqcap^{S(0)} = \mathrm{Tr}_B\, \omega_\sqcap^{(0)} = \sum_{k=1}^{d_S} p_k |E_k^S\rangle\langle E_k^S| \,, \tag{17}$$

with

$$p_k = \frac{\Omega_\Delta^B(E - E_k^S)}{\sum_k \Omega_\Delta^B(E - E_k^S)} \,. \tag{18}$$

Here, $\Omega_\Delta^B(E - E_k^S)$ denotes the number of states of the bath with an energy contained in the interval $[E-E_k^S, E-E_k^S+\Delta]$. For simplicity we assume that $\|H_S\|_\infty \leq E$. Notice that the probabilities $\{p_k\}$ only depend on the shape of the spectrum of the bath. We aim at bounding the trace distance

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho^S_{\rm Gibbs}) = \frac{1}{2}\sum_k |p_k - q_k| \,, \tag{19}$$

where $\{q_k\}$ are the probabilities of the Gibbs state in its eigenbasis,

$$q_k = \frac{\mathrm{e}^{-\beta E_k^S}}{Z_Q} \,, \tag{20}$$

with $Z_Q = \sum_i \mathrm{e}^{-\beta E_i^S}$.

Let us define a function S as the logarithm of the number of states of the bath

$$S(E) = \log \Omega_\Delta^B(E) \,. \tag{21}$$

The Hilbert space of the bath is finite dimensional and thus the spectrum of the bath is discrete, from now on it is however assumed that the bath is large enough such that $S : \mathbb{R}^+ \to \mathbb{R}^+$ can be well approximated by a twice differentiable function $s : \mathbb{R}^+ \to \mathbb{R}^+$. For natural systems and reasonable energy ranges the additional error from this approximation is exponentially small in the size of the bath. For the sake of conciseness we ignore such exponentially small errors. We discuss this continuous approximation more closely in Appendix B.

From now on we will hence focus on $s(E) = \log \Xi_\Delta^B(E)$, where Ξ_Δ^B it the smooth approximation of Ω_Δ^B. Taylor's theorem ensures that for every k there exists some $\xi_k \in [E - E_k^S, E]$, such that

$$\begin{aligned} s(E - E_k^S) &= s(E) - \frac{\partial s}{\partial E}(E) E_k^S + \frac{\partial^2 s}{\partial E^2}(\xi_k) {E_k^S}^2 \\ &= s(E) - \beta E_k^S + \gamma_k \,, \end{aligned} \tag{22}$$

where

$$\beta = \frac{\partial s}{\partial E}(E) \tag{23}$$

is the inverse temperature and

$$\gamma_k = \frac{\partial^2 s}{\partial E^2}(\xi_k)(E_k^S)^2. \tag{24}$$

A linear expansion of s is equivalent to an exponential fit of the smoothed number of states of the bath $\Xi_\Delta^B(E - E_k^S)$,

$$\Xi_\Delta^B(E - E_k^S) = \mathrm{e}^{s(E)-\beta E_k^S+\gamma_k} \ . \tag{25}$$

Thus, the probabilities $\{p_k\}$ can be written as

$$p_k = \frac{\Xi_\Delta^B(E - E_k^S)}{\sum_i \Xi_\Delta^B(E - \varepsilon_i)} = \frac{\mathrm{e}^{-\beta E_k^S+\gamma_k}}{Z_P} \, , \tag{26}$$

where $Z_P = \sum_i \mathrm{e}^{-\beta\varepsilon_i+\gamma_i}$. Therefore, the distance between $\omega_\sqcap^{S(0)}$ and the Gibbs state depends on how well the density of states of the bath is approximated by an exponential curve. The difference between the probabilities reads

$$p_k - q_k = \underbrace{\frac{\mathrm{e}^{-\beta E_k^S}}{Z_Q}}_{q_k} \left(\frac{Z_Q}{Z_P} \, \mathrm{e}^{\gamma_k} - 1 \right) \, , \tag{27}$$

where the fraction Z_Q/Z_P can be rewritten as

$$\frac{Z_Q}{Z_P} = \sum_k \frac{\mathrm{e}^{-\beta E_k^S+\gamma_k}}{Z_P} \, \mathrm{e}^{-\gamma_k} = \sum_k p_k \, \mathrm{e}^{-\gamma_k} \ . \tag{28}$$

Introducing the notation

$$\gamma_{\min} = \min_k \min_{\xi_k \in [E-E_k^S, E]} \gamma_k(\xi_k) \tag{29}$$

$$\gamma_{\max} = \max_k \max_{\xi_k \in [E-E_k^S, E]} \gamma_k(\xi_k) \tag{30}$$

we can write

$$\begin{aligned} |p_k - q_k| &= q_k \left| \left(\sum_k p_k \, \mathrm{e}^{-\gamma_k} \right) \mathrm{e}^{\gamma_k} - 1 \right| \\ &\leq q_k \left(\mathrm{e}^{\gamma_{\max}-\gamma_{\min}} - 1 \right) \, . \end{aligned} \tag{31}$$

The trace distance between the reduced dephased decoupled rectangular state $\omega_\sqcap^{S(0)}$ and the Gibbs state is thus bounded from above by

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S) \leq \frac{1}{2} \left(\mathrm{e}^{\gamma_{\max}-\gamma_{\min}} - 1 \right) + C \, , \tag{32}$$

where C is exponentially small in the bath size. We explicitly bound $\gamma_{\max} - \gamma_{\min}$ for a specific bath in Appendix B.

B Reduced density matrix of the dephased rectangular decoupled state – a specific model

In order to have a more explicit expression for (32) let us consider a particular model for the bath. We will also use this bath for the algorithm presented in the last part of the article.

We start with the natural choice of m non-interacting uncoupled spin-$1/2$ particles with energies 0 and η. The spectrum of this model is discrete and energy can take integer values between 0 and $\|H_B\|_\infty = \eta m$. The system is highly degenerate and the number of states with energy k follows a binomial distribution $\binom{m}{k}$.

This degeneracy makes it impossible to find a sufficiently good smooth approximation $\Xi_\Delta^B(E)$ for the number of states $\Omega_\Delta^B(E)$ such that even for intervals whose width Δ scales like a $d^{-\kappa}$ with $0 < \kappa < 1$ the error in the approximation of the local density $(\Xi_\Delta^B(E) - \Omega_\Delta^B(E))/d$ goes to zero for large d. That is, the continuous approximation would cause additional errors that would not go down exponentially fast with the bath size.

Therefore we need to assume that the degeneracy of the levels are lifted by a suitable perturbation. As we are only concerned about the spectrum and not the eigenstates of the bath basically any perturbation of adequate strength, such as a basically arbitrary weak interaction, will be sufficient to do this, such that this is not a problem for implementations. A convenient way to perturb the model for a theoretical study is to replace the fixed local field strength by a normal distributed random field strength such that on average the energy of the local excited state is still η above the local ground state. If the width of the normal distribution is chosen in a suitable way, instead of the degenerate subspaces with energies at integer multiples of η we get, with overwhelmingly high probability, a density of states that can be well approximated by

$$\varrho(E') = \frac{1}{\eta} 2^m \left(\frac{2}{\pi m} \right)^{1/2} \mathrm{e}^{-2m(\frac{E'}{\eta m} - \frac{1}{2})^2} \tag{33}$$

in the aforementioned sense.

Hence, the smoothed number of states in the interval $[E, E + \Delta]$ is given by

$$\Xi_\Delta^B(E) = \int_E^{E+\Delta} \varrho(E') \mathrm{d}E' \, . \tag{34}$$

Our aim is to bound $\gamma_{\max} - \gamma_{\min}$ in Eq. (32) for this model. To do this, we first consider the case when $\Delta \ll \|H_B\|_\infty$, such that

$$\Xi_\Delta^B(E) \simeq \frac{\Delta}{\eta} 2^m \left(\frac{2}{\pi m} \right)^{1/2} \mathrm{e}^{-2m(\frac{E'}{\eta m} - \frac{1}{2})^2} \ . \tag{35}$$

We can easily compute the second derivative of the logarithm of the above expression and find

$$\frac{\partial^2 s}{\partial E^2} = -\frac{4}{\eta^2 m} \, . \tag{36}$$

If Δ is not much smaller than $\|H_B\|_\infty$, $s(E)$ deviates from the parabolic form. But, larger Δ only make the curvature of $s(E)$ smaller. In general we have

$$0 > \frac{\partial^2 s}{\partial E^2} > -\frac{4}{\eta^2 m} \, , \tag{37}$$

and thus $\gamma_{\max} - \gamma_{\min} \leq \gamma_{\max} \leq 4\|H_S\|_\infty^2/(\eta^2 m)$ so that

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\text{Gibbs}}^S) \leq \frac{1}{2}\left(\mathrm{e}^{4\frac{\|H_S\|_\infty^2}{\eta^2 m}} - 1\right) + C, \tag{38}$$

where C is exponentially small in the bath size. In natural situations the right hand side of the above equation will be very small as $\|H_S\|_\infty^2 \ll \eta^2 m$.

The rectangular states are a quite artificial class of states. So what happens if instead of $\omega_\sqcap^{S(0)}$ we take states with a different energy distribution? Will we still get something close to a Gibbs state as long as the width of the energy distribution is not to small and the density of states is exponentially increasing? The exponential increase in the density of states ensures that most of the contribution to $\omega_\sqcap^{(0)}$ comes from the upper edge of the interval $E + \Delta$ in the case of a rectangular distribution. Thus, it can be expected that one will get a state that is close to a Gibbs state for any energy distribution that is sufficiently smooth, and has a sufficiently sharp cutoff to higher energies. Where by sufficiently sharp we mean that it must drop from a value much larger than $1/d$ to a value much smaller than $1/d$ in an energy interval that is small compared to $(\partial^2 s/\partial E^2)^{-1/2}$. The smoothness is required as for certain systems that violate the so called *eigenstate thermalization hypothesis* (ETH) [14] details of the energy distribution can have a huge impact on certain properties of the state. That smoothness of the energy distribution is required to guarantee thermalization in such systems can be seen for example in the model studied in [9].

C Complexity of the algorithm at low temperatures

In this section, we discuss how the number of times the algorithm must be repeated before the energy window corresponding to the desired temperature is hit depends in the temperature. As we are only interested in the number of repetitions we can assume that the algorithm runs "perfectly" in that it generates exactly a rectangular state with fixed width Δ at some position E of the spectrum. Furthermore we are only interested in cases where the reduced state of the rectangular state can be guaranteed to be close to a Gibbs state, i.e., we may assume that the spectrum of the bath is dense enough such that the number of states of the bath in the interval $[E, E + \Delta]$, can be to well approximated by a continuous, twice differential function $\Xi_\Delta^B(E)$ that increases exponentially to higher energies.

The probability of getting a position E is given by

$$P(E) = \frac{\Xi_\Delta(E)}{d} = \frac{1}{d}\sum_{k=1}^{d_S} \Xi_\Delta^B(E - E_k^S)\,, \tag{39}$$

Using that the density of states of the bath can be locally approximated by an exponential we obtain

$$P(E) \approx \frac{1}{d}\sum_{k=1}^{d_S} \mathrm{e}^{-\beta E_k^S}\, \Xi_\Delta^B(E)\,. \tag{40}$$

Then, the probability of attaining a position E can be bounded from above by

$$P(E) \approx \frac{1}{d_S}\sum_{k=1}^{d_S} \mathrm{e}^{-\beta E_k^S}\, P_\Delta^B(E) \leq \mathrm{e}^{-\beta E_1^S}\, P_\Delta^B(E) \leq \mathrm{e}^{-\beta E_1^S}\,, \tag{41}$$

with $P_\Delta^B(E) = \Xi_\Delta^B(E)/d_B \leq 1$ and E_1^S the gap of the system. The number of times that the program must be run on average in order to get the rectangular state at the position E is thus lower bounded by

$$\overline{\sharp \text{ runs}} \approx \frac{1}{P(E)} \geq \mathrm{e}^{\beta E_1^S}\,. \tag{42}$$

This last equation shows that generically, it is exponentially hard to go to low temperatures. This is to be expected, of course, as no structure of the Hamiltonian is being used, and generic local Hamiltonian systems can presumably not be efficiently cooled to arbitrarily close to their ground state (which would then efficiently solve QMA-hard problems on a quantum computer [20]). Needless to say, for specific Hamiltonians, with some additional structure, an algorithm can well be more efficient. The coefficient of the exponential is related to the features of the spectrum at low energies. In the case in which there is a gap the ground state could encode the solution of a satisfiability problem that is expected to be a hard problem.

D Temperature and error in the temperature for the bath described in Appendix A

In order to give an explicit expression for $\mathcal{D}(\omega_{QC}, \omega_\sqcap)$, the density of states of the total system (system + bath) is required. Although the density of states of the subsystem is completely unknown (the Hamiltonian of the system is a black box for us), if the a particular model for the bath is taken, it is still possible to give a bound for $\mathcal{D}(\omega_{QC}, \omega_\sqcap)$ in terms of the operator norm $\|H_S\|_\infty$.

If we take all possible exchanges of energy between the system and bath into account, but treat them together as a closed system, the density of states of the whole set can be generally written as

$$\varrho(E) = \sum_{k=1}^{d_S} \varrho_B(E - E_k^S) \tag{43}$$

where E_k^S are the energies of the system and the assumption $E \geq \|H_S\|_\infty$ has been used.

Next, let us consider the bath described in Appendix B. The main motivation to focus on such a model – apart from it being physically very plausible as an approximation to very weakly coupled quantum systems – is its efficient simulability and the fact that its density of states can be very well locally aproximated by an exponential curve. In particular, the smooth density of states of the bath reads

$$\varrho_B(E) = d_B \frac{1}{\eta}\left(\frac{2}{\pi m}\right)^{1/2} \mathrm{e}^{-2m\left(\frac{E}{\eta m} - \frac{1}{2}\right)^2}\,, \tag{44}$$

where $d_B = 2^m$ is the dimension of the Hilbert space of the bath, η is the energy unit of one excitation, m is the number of qubits of the bath register, and $0 \leq E < \|H_B\|_\infty = \eta m$.

After running the algorithm, a state close to the rectangular state is obtained at the position $E = \tilde{\varphi}\|H\|_\infty$ of the spectrum. The system is then thermalized at an inverse temperature

$$\begin{aligned}\beta &= \frac{\mathrm{d}\ln \Xi_\Delta^B(E)}{\mathrm{d}E} = \frac{4}{\eta}\left(\frac{1}{2} - \frac{E}{\eta m}\right) \\ &= \frac{4}{\eta}\left(\frac{1}{2} - \tilde{\varphi}\left(1 + \frac{\|H_S\|_\infty}{\|H_B\|_\infty}\right)\right). \end{aligned} \tag{45}$$

In practice, β is an input of our algorithm and, both the number of qubits of the ancilla register r and the number of qubits q that are measured in the end, are parameters that must be determined before running the circuit. The algorithm will be run repeatedly until the value $\tilde{\varphi}$ corresponding to the desired β is obtained. For the density of states considered here, this value $\tilde{\varphi}$ is

$$\tilde{\varphi} = \frac{1}{1 + \frac{\|H_S\|_\infty}{\|H_B\|_\infty}}\left(\frac{1}{2} - \frac{\eta\beta}{4}\right). \tag{46}$$

It follows from Eq. (46) that

$$\delta\beta \leq \frac{4c}{\eta}\left(1 + \frac{\|H_S\|_\infty}{\|H_B\|_\infty}\right), \tag{47}$$

as $c = 2^{-q}$, to reach a given precision $\delta\beta$ in the temperature it is sufficient to choose

$$q = \left\lceil \log_2 \frac{\|H\|_\infty}{\Delta} \right\rceil = \left\lceil -\log_2\left(\frac{\eta\delta\beta}{1 + \frac{\|H_S\|_\infty}{\|H_B\|_\infty}}\right) + 2 \right\rceil. \tag{48}$$

E Error and average number of runs of the quantum algorithm

In this section the error of the quantum algorithm is derived and a bound on the average number of repetitions that are necessary to reach the desired energy is given. The error

$$\varepsilon = \mathcal{D}(\omega_{QC}^S, \rho_{\mathrm{Gibbs}}^S) \leq \mathcal{D}(\omega_{QC}, \omega_\sqcap^{(0)}) + \mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S) \tag{49}$$

consists of two components. The deviation of the reduced rectangular state from the Gibbs state $\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S)$ that has been calculated in Appendix A and B. In the following we bound the deviation of the final sate of the algorithm from the rectangular state $\mathcal{D}(\omega_{QC}, \omega_\sqcap^{(0)})$. Again we start by considering general baths and then derive a more explicit expression for the bath described in Appendix B. The main problem that we will have to deal with while bonding $\mathcal{D}(\omega_{QC}, \omega_\sqcap^{(0)})$ is that the density of states of the bath is highly non uniform. The partial phase estimation procedure prepares a state whose energy distribution is very close to a rectangular energy distribution, but due to the highly non uniformity of the density of states this is not sufficient to guarantee a good approximation to a rectangular state. Although the partial phase estimation yields a state whose energy distribution becomes, in one norm, exponentially close to rectangular by increasing r a polynomially large number of ancilla qubits is necessary to ensure a small trace norm error from the rectangular state as the main contribution to the error comes form the extremely dense part of the spectrum even though there the approximately rectangular energy distribution is almost zero. This is a general problem of quantum phase estimation and not particular to our algorithm.

We will see that the bounds on the two contributions that we will find for the bath discussed in Appendix B

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S) \leq \frac{1}{2}\left(\mathrm{e}^{4\frac{\|H_S\|_\infty^2}{\eta^2 m}} - 1\right) + C \tag{50}$$

$$\begin{aligned}\mathcal{D}(\omega_{QC}, \omega_\sqcap) \leq\ & \mathrm{e}^{\frac{2\|H_S\|_\infty^2}{\eta^2 m} + \beta\|H_S\|_\infty + \frac{\eta^2 m\beta^2}{8}} \\ & \times 2^{q-r+2}\left(1 + \ln(2^{r-q})/\pi^2\right) + C\end{aligned} \tag{51}$$

(again C is exponentially small in the bath size) depend on the energy unit η of the bath. It is convenient to write η in term of a dimensionless parameter $\lambda > 0$

$$\eta = \left(\frac{\lambda}{m}\right)^{1/2}\|H_S\|_\infty, \tag{52}$$

because then the two errors can be written in the form:

$$\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S) \leq \frac{1}{2}(\mathrm{e}^{\frac{4}{\lambda}} - 1) + C \tag{53}$$

$$\begin{aligned}\mathcal{D}(\omega_{QC}, \omega_\sqcap) \leq\ & \mathrm{e}^{\frac{2}{\lambda} + \beta\|H_S\|_\infty + \frac{\lambda\|H_S\|_\infty^2\beta^2}{8}} \\ & \times 2^{q-r+2}\left(1 + \ln(2^{r-q})/\pi^2\right) + C\end{aligned} \tag{54}$$

To reduce the trace distance $\mathcal{D}(\omega_\sqcap^{S(0)}, \rho_{\mathrm{Gibbs}}^S)$ it is favorable to choose a large λ. Intuitively this captures the fact that the energy content in the bath must be much larger than that of the system in order to get a Gibbs state. However, this also increases the error in the approximation of the rectangular state by the algorithm because phase estimation on a system with a more dense spectrum is harder. This increase of the error can however be compensated by increasing the accuracy of the phase estimation by linearly increasing the number of qubits r in the ancilla register. Similarly lower temperatures can be reached by a quadratic increase of the number of ancilla qubits of order $O(\beta^2\|H_S\|_\infty^2)$. As the phase estimation however requires a total number of 2^r controlled unitary operations this comes at an exponential cost in terms of runtime. This is expected to be a general feature of all algorithms using phase estimation on many particle systems.

Before we go into the derivation of $\mathcal{D}(\omega_{QC}, \omega_\sqcap)$ let us quickly calculate the average number of runs that are required to get a certain temperature for the bath discussed in Appendix B in terms of λ. From Eqs. (39) and (42) and the explicit formula for the smoothed number states given in (76) it is easy to see that

$$\overline{\sharp\,\text{runs}} \leq \sqrt{\frac{\pi\lambda}{2}}\frac{\|H_S\|_\infty}{\Delta}\,\mathrm{e}^{\frac{2}{\lambda} + \beta\|H_S\|_\infty + \frac{\lambda\|H_S\|_\infty^2\beta^2}{8}}. \tag{55}$$

Deviation from the rectangular state for a general bath

The trace distance between the state generated by the circuit ω_{QC} and and the rectangular state $\omega_{\sqcap}$ can be written in terms of the one norm distance of the distributions of the diagonal elements

$$\mathcal{D}(\omega_{QC},\omega_{\sqcap}) = \frac{1}{2}\sum_{k=1}^{d} |q_k - p_k| \ , \tag{56}$$

where the $\{q_k\}$ and $\{p_k\}$ are the eigenvalues of ω_{QC} and $\omega_{\sqcap}$ respectively. These probability distributions can be defined as

$$q_k = \frac{F_N(\varphi_k - \tilde{\varphi})}{Z_F}, \tag{57}$$

$$p_k = \frac{G(\varphi_k - \tilde{\varphi})}{Z_G} \, , \tag{58}$$

where $\varphi_k = E_k/\|H\|_\infty$ are the phases corresponding to the eigenvalues of the Hamiltonian, $Z_F = \sum_{j=1}^{d} F_N(\varphi_j - \tilde{\varphi})$ and $Z_G = \sum_{j=1}^{d} G(\varphi_j - \tilde{\varphi})$ are normalization constants, and the functions F_N and G read

$$F_N(\varphi) = \frac{1}{cN}\sum_{k=0}^{cN} f_N\left(\varphi - \frac{k}{N}\right) \tag{59}$$

$$G(\varphi) = \frac{1}{c}\left(\Theta(\varphi) - \Theta(\varphi - c)\right) \, , \tag{60}$$

with

$$f_N(\varphi) = N|\alpha_0(\varphi)|^2 = \frac{1}{N}\frac{\sin^2(\pi N\varphi)}{\sin^2(\pi\varphi)}, \tag{61}$$

$N = 2^r$, $c = \Delta/\|H\|_\infty = 2^{-q}$ the relative width of the energy interval and Θ the step function (see main text). The phase $\tilde{\varphi} = s_*/2^q$ stands for the position of the rectangular state in the spectrum ($E = \tilde{\varphi}\|H\|_\infty$), where s_* is the outcome of the measurement and q the number of measured qubits. The phases $\varphi_k = E_k/\|H\|_\infty$ and therefore $0 \leq \varphi_k < 1$ for any k. Notice that both F_N and f_N are periodic functions with period 1, although they are obviously only considered in the interval $[0,1[$. Both distributions are normalized on this interval.

It is easy to see that Eq. (56) is bounded by

$$\mathcal{D}(\omega_{QC},\omega_{\sqcap}) \leq \frac{1}{Z_G}\sum_{k=1}^{d} |F_N(\varphi_k - \tilde{\varphi}) - G(\varphi_k - \tilde{\varphi})| \ . \tag{62}$$

Notice that $Z_G = \Omega_\Delta(E)/c$, where $\Omega_\Delta(E)$ is the number of states in the interval $[E, E+\Delta]$.

The main problem to estimate Eq. (62) is that both the spectrum of the system and the spectrum of the bath are unknown. Nevertheless, considering that the spectrum of the whole system is sufficiently dense it is possible to approximate the upper bound in Eq. (62) by an integral. With this aim, let us decompose the sum (62) into bins of width $\|H\|_\infty/L$

$$\mathcal{D}(\omega_{QC},\omega_{\sqcap}) \leq \sum_{i=0}^{L-1} \sum_{E_k \in \left[\frac{j}{L},\frac{j+1}{L}\right[} h(E_k) \, , \tag{63}$$

where,

$$h(E') = \frac{1}{Z_G}\left| F_N\left(\frac{E'}{\|H\|_\infty} - \tilde{\varphi}\right) - G\left(\frac{E'}{\|H\|_\infty} - \tilde{\varphi}\right)\right| , \tag{64}$$

is a function introduced to simplify the notation and L is the number of bins in which the spectrum has been divided. The idea here is to take an L as large as possible. The only one restriction that has to be taken into account is that the number of energy values in a bin, $\Omega_{\|H\|_\infty/L}(j\|H\|_\infty/L)$, can be well approximated by its continuous version $\Xi_{\|H\|_\infty/L}(j\|H\|_\infty/L)$ (compare the discussion of the continuous approximation in Appendix B). For a bath with a continuous form for the number of states $\Xi_\Delta(E)$, it is always possible to take an L proportional to the dimension of the Hilbert space d or, at least, to some power d^κ with $0 < \kappa < 1$. Thus, L scales exponentially with the size of the bath.

As h is a differentiable function, Taylor's theorem ensures that for every bin j there exist some value $\xi_j \in [j\|H\|_\infty/L, (j+1)\|H\|_\infty/L[$ for which

$$h(E_k) = h\left(\frac{j\|H\|_\infty}{L}\right) + h'(\xi_j)\left(E_k - \frac{j\|H\|_\infty}{L}\right) \, , \tag{65}$$

where $j\|H\|_\infty/L \leq E_k < (j+1)\|H\|_\infty/L$. Then, the contribution of the j-th bin in Eq. (63) can be bounded from above by

$$\sum_{E_k \in \left[\frac{j}{L},\frac{j+1}{L}\right[} h(E_k) \leq \Omega_{\frac{\|H\|_\infty}{L}}\left(\frac{j\|H\|_\infty}{L}\right) \times \left(h\left(\frac{j\|H\|_\infty}{L}\right) + \sup_{\xi_j \in \left[\frac{j}{L},\frac{j+1}{L}\right[} h'(\xi)\frac{\|H\|_\infty}{L}\right) . \tag{66}$$

The last term in the parenthesis in Eq. (66) decreases with L and thus is exponentially small in the bath size. This can be verified with a lengthy, but straightforward calculation. The main contribution to the error of the circuit is given by the product $\Omega\, h$. The same is true for the approximation of $\Xi_\Delta(E)$ by $\Omega_\Delta(E)$, its error is negligible with respect to the bound given by Eq. (66).

In order to transform Eq. (63) into an integral, let us again introduce the density of states from the continuous number of states $\Xi_\Delta(E)$,

$$\varrho(E') = \lim_{\delta\to 0}\frac{\Xi_\delta(E')}{\delta} \, . \tag{67}$$

The number of states can then be written in terms of the density of states as

$$\Omega_\delta\left(E'\right) = \varrho\left(E'\right)\delta + O(\delta^2) \, . \tag{68}$$

Putting Eqs. (63), (66) and (68) together, the error of the circuit can be bounded from above by

$$\mathcal{D}(\omega_{QC},\omega_{\sqcap}) \leq \sum_{i=0}^{L-1} h\left(\frac{i\|H\|_\infty}{L}\right)\varrho\left(\frac{i\|H\|_\infty}{L}\right)\frac{\|H\|_\infty}{L} + O\left(L^{-1}\right) \, . \tag{69}$$

Notice that the upper bound of the previous equation converges to an integral for $L \to \infty$ with deviations that scale as $O(L^{-1})$. Thus, the trace distance between ω_{QC} and $\omega_{\sqcap}$ is bounded from above by

$$\mathcal{D}(\omega_{QC}, \omega_{\sqcap}) \leq \|h\, \varrho\|_1 + O\left(L^{-1}\right) , \tag{70}$$

where

$$\|h\, \varrho\|_1 = \int_0^{\|H\|_\infty} \mathrm{d}E' h\left(E'\right) \varrho(E') . \tag{71}$$

We will bound $\|h\, \varrho\|_1$ for the model described in Appendix B in the next section.

Deviation from the rectangular state for the bath described in Appendix B

Next, the error of the circuit for a bath as described in Appendix A is bounded. In particular, Eq. (70) is bounded for a bath with the density of states given by Eq. (44). The one norm $\|h\, \varrho\|_1$ can be trivially bounded by

$$\|h\, \varrho\|_1 \leq \frac{c}{\Xi_\Delta(E)} \|F_N - G\|_1 \sup_{0 \leq E' \leq \|H\|_\infty} \varrho(E') , \tag{72}$$

where the definition of h given in (64) has been used. If the density of states $\varrho(E)$, defined in Eq. (43), is written in terms of the inverse temperature given in Eq. (45),

$$\begin{aligned} \varrho(E) = \sum_{k=1}^{d_S} \mathrm{e}^{-\frac{2(E_k^S)^2}{\eta^2 m}} \mathrm{e}^{-\beta E_k^S} \\ \times d_B \frac{1}{\eta} \left(\frac{2}{\pi m}\right)^{1/2} \mathrm{e}^{-\eta^2 m \beta^2/8} , \end{aligned} \tag{73}$$

it is easy to see that its maximum value corresponds to $\beta = 0$ (We only consider positive temperatures here) and the supremum can be bounded by

$$\sup_{0 \leq E' \leq \|H\|_\infty} \varrho(E') \leq \frac{d}{\eta} \left(\frac{2}{\pi m}\right)^{1/2} , \tag{74}$$

where $d = d_S d_B$ is the dimension of the Hilbert space of the total system. Then, the one norm of $\|h\, \varrho\|_1$ is bounded from above by

$$\|h\, \varrho\|_1 \leq \frac{c}{\Xi_\Delta(E)} \frac{d}{\eta} \left(\frac{2}{\pi m}\right)^{1/2} \|F_N - G\|_1 . \tag{75}$$

To give a more explicit expression, the number of states $\Xi_\Delta(E)$ can be lower bounded by

$$\begin{aligned} \Xi_\Delta(E) &= \int_E^{E+\Delta} \varrho(E') \mathrm{d}E' \geq \varrho(E)\Delta \\ &\geq \frac{\Delta d}{\eta} \left(\frac{2}{\pi m}\right)^{1/2} \mathrm{e}^{\frac{-2\|H_S\|_\infty^2}{\eta^2 m} - \beta\|H_S\|_\infty - \frac{\eta^2 m \beta^2}{8}} , \end{aligned} \tag{76}$$

where it has been assumed that E is in a position of the spectrum with positive temperature and therefore $\varrho(E)$ is an increasing function. Then, the trace distance $\mathcal{D}(\omega_{QC}, \omega_{\sqcap})$ is bounded by

$$\begin{aligned} \mathcal{D}(\omega_{QC}, \omega_{\sqcap}) \leq \mathrm{e}^{\frac{2\|H_S\|_\infty^2}{\eta^2 m} + \beta\|H_S\|_\infty + \frac{\eta^2 m \beta^2}{8}} \frac{\|F_N - G\|_1}{\|H\|_\infty} \\ + O(L^{-1}) . \end{aligned} \tag{77}$$

In order for this error to become small the one norm $\|F_N - G\|_1$ must be made small enough such that it compensates the exponential prefactors. As we will see in the next section this can be achieved by using a polynomially large ancilla register R.

One norm between F_N and G

The one norm between F_N and G is defined as

$$\|F_N - G\|_1 = \int_0^{\|H\|_\infty} \left| F_N\left(\frac{E'}{\|H\|_\infty}\right) - G\left(\frac{E'}{\|H\|_\infty}\right) \right| \mathrm{d}E' , \tag{78}$$

where F_N and G are defined in (59) and (60). By a simple change of variables it is easy to show that

$$\frac{\|F_N - G\|_1}{\|H\|_\infty} = \int_0^1 |F_N(\varphi) - G(\varphi)| \, \mathrm{d}\varphi , \tag{79}$$

Remember that both $F_N(\varphi)$ and $G(\varphi)$ are normalized on the interval $[0, 1]$ and that $G(\varphi)$ is a step function that is non-zero only in the interval $[0, c[$ and that in this interval $F_N(\varphi) < G(\varphi) = 1/c$. Using this, the previous integral can be rewritten as

$$\begin{aligned} \frac{\|F_N - G\|_1}{\|H\|_\infty} &= 2 \int_c^1 \mathrm{d}\varphi F_N(\varphi) \\ &= \frac{2}{cN} \sum_{k=0}^{cN} \int_c^1 \mathrm{d}\varphi\, f_N\left(\varphi - \frac{k}{N}\right) . \end{aligned} \tag{80}$$

Due to the symmetry and periodicity of f_N, the contribution to the previous integral of the right tail of $f_N(\varphi - k/N)$ is the same as the contribution of the left tail of $f_N(\varphi - (c - k/N))$ for $k/N \leq c$,

$$\int_c^{\frac{k}{N}+\frac{1}{2}} \mathrm{d}\varphi\, f_N\left(\varphi - \frac{k}{N}\right) = \int_{c-\frac{k}{N}+\frac{1}{2}}^1 \mathrm{d}\varphi\, f_N\left(\varphi - c + \frac{k}{N}\right) .$$

This implies that

$$\frac{\|F_N - G\|_1}{\|H\|_\infty} = \frac{4}{cN} \sum_{k=0}^{cN} \int_c^{\frac{k}{N}+\frac{1}{2}} \mathrm{d}\varphi\, f_N\left(\varphi - \frac{k}{N}\right) . \tag{81}$$

The integral of the previous equation can be bounded by

$$\int_c^{\frac{k}{N}+\frac{1}{2}} \mathrm{d}\varphi\, f_N\left(\varphi - \frac{k}{N}\right) \leq \frac{\cot\left(\pi(c - k/N)\right)}{\pi N} , \tag{82}$$

where the bound

$$f_N\left(\varphi-\frac{k}{N}\right)\leq\frac{1}{N\sin^2\left(\varphi-\frac{k}{N}\right)} \tag{83}$$

has been used. Therefore, the distance between the functions F_N and G can be bounded by

$$\frac{\|F_N-G\|_1}{\|H\|_\infty}\leq\frac{4}{cN}\left(\frac{1}{2}+\sum_{k=0}^{cN-1}\frac{\cot\left(\pi(c-k/N)\right)}{\pi N}\right), \tag{84}$$

where the sum has been split up in the $k=cN$ case, which is exactly $1/2$, and the rest. The sum of the previous equation can be bounded in two steps by

$$\begin{aligned}\sum_{k=1}^{cN}\frac{\pi}{N}\cot\left(\frac{\pi k}{N}\right)&\leq\frac{\pi}{N}\cot\left(\frac{\pi}{N}\right)+\int_{\frac{1}{N}}^{c}\mathrm{d}u\cot(\pi u)\\&\leq 1+\ln\left(cN\right).\end{aligned} \tag{85}$$

Thus, the one norm between F_N and G is bounded by

$$\frac{\|F_N-G\|_1}{\|H\|_\infty}\leq\frac{4}{\pi^2}\frac{1}{cN}\left(\frac{\pi^2}{2}+1+\ln(cN)\right), \tag{86}$$

where as before $N=2^r$, $c=\Delta/\|H\|_\infty=2^{-q}$. Inserting this into (77) we get

$$\begin{aligned}\mathcal{D}(\omega_{QC},\omega_\sqcap)\leq\,&\mathrm{e}^{\frac{2\|H_S\|_\infty^2}{\eta^2 m}+\beta\|H_S\|_\infty+\frac{\eta^2 m\beta^2}{8}}\\&\times 2^{q-r+2}\left(1+\ln(2^{r-q})/\pi^2\right)\end{aligned} \tag{87}$$

up to errors exponentially small in the bath size. This completes the discussion of an upper bound of the error made in the quantum algorithm.

F Discussion of the argument presented in Ref. [17]

Ref. [17] presents a novel approach towards thermalizing quantum systems using an iterative approach, in which prethermalized parts are put together in a suitable fashion in order to arrive at a Gibbs state of a quantum system with a local Hamiltonian. This argument provides a new intuition on how one can think of thermalizing local quantum systems, different from a quantum Monte Carlo approach (and the one presented here). In this appendix, however, we point out a quite serious challenge that seem to have to be overcome to make such an argument fully rigorous. The authors of Ref. [17] are aware of, and have acknowledged the existence of, this challenge.

Each merging step consists of two steps. The first is a probabilistic step that updates the probability weights of the Gibbs state by means of postselection. The second one aims at rotating the eigenbasis of the old Hamiltonian to the one of the new Hamiltonian by means of an instance of dephasing. Each step has as an input a chosen $\varepsilon>0$, and for the entire algorithm to work, this procedure has to be correct up to errors of $O(\varepsilon)$. In what follows, we refer to the equation numbering of the preprint v2.

In Eq. (5), perfect dephasing is being achieved when $\sigma\to\infty$ is taken. This is approximated by imperfect dephasing based on a choice of a finite σ. From the Dyson series of second order (6)-(8), it follows that (in the asymptotic notation)

$$\sigma=O(1/\varepsilon). \tag{88}$$

This is not made explicit in the paper, but appears to be crucial. Intuitively speaking, if σ becomes larger, the dephasing is more exact, but then (6)-(8) can no longer be used.

This step is then used in the procedure following Eq. (13). A ζ is introduced and dephasing between eigenstates with relative gap larger than ζ is considered. Then a new Hamiltonian $\tilde{H}$ is constructed that has this feature: It has the same eigenbasis as $H+\varepsilon h$, but with eigenvalues grouped in bins, such that the smallest gap between bins is ζ. For the following procedure to work, one has to take (again in the asymptotic notation)

$$\sigma=\theta(1/\zeta), \tag{89}$$

so both $\sigma=O(1/\zeta)$ and $\sigma=\Omega(1/\zeta)$ (although only $\sigma=O(1/\zeta)$ is made explicit, both bounds are actually needed).

This, however, seems to already fix $\zeta=\Omega(\varepsilon)$. So there is no longer the freedom to have

$$\zeta=\varepsilon^2\beta\|h\|^2, \tag{90}$$

which would mean that $\zeta=\theta(\varepsilon^2)$. This appears to contradict the above statement. Again, intuitively, σ is "forced to be small for the Dyson approach to work", but at the same time this gives a constraint to ζ which then "implies σ to be large". It seems challenging to combine these apparently contradictory constraints in a fully rigorous argument, although this might well be possible.

G Theorem 1 for an exponential density of states

As we have seen in the main text in theorem 1 the distinguishability of the microcanonical states $\omega_\sqcap^{(0)}$ and $\omega_\sqcap$ corresponding to an interval $[E,E+\Delta]$ of the Hamiltonians H_0 and $H=H_0+V$ is bounded by

$$\mathcal{D}(\omega_\sqcap^S,\omega_\sqcap^{S(0)})\leq\mathcal{D}(\omega_\sqcap,\omega_\sqcap^{(0)})\leq\frac{\|V\|_\infty}{\varepsilon}+\frac{\Delta\Omega+\Omega_\varepsilon}{2\,\Omega_{\min}}, \tag{91}$$

where $\Omega_{\min}$ and $\Delta\Omega$ are the minimum, and the difference, of the dimensions of the support of $\omega_\sqcap^{(0)}$ and $\omega_\sqcap$, and Ω_ε is the total number of eigenstates of H and H_0 in the intervals $[E,E+\varepsilon]$ and $[E+\Delta-\varepsilon,E+\Delta]$.

In the main text, in order to give a more comprehensible interpretation to Eq. (91), an approximately constant density of states was assumed and it was shown that

$$\mathcal{D}(\omega_\sqcap^S,\omega_\sqcap^{S(0)})\lessapprox\frac{3\sqrt{2}}{2}\left(\frac{\|V\|_\infty}{\Delta}\right)^{1/2}. \tag{92}$$

Nevertheless, we have seen that thermal states emerge in situations where the density of states is locally well approximable by an exponential, and therefore, the assumption of uniform density of states is not true anymore. Thus, new conditions that ensure the indistinguishability of the microcanonical states $\omega_\sqcap^S$ and $\omega_\sqcap^{S(0)}$ must be derived for the exponential density of states

$$\varrho(E) = \frac{\mathrm{d}\Xi_\Delta(E)}{\mathrm{d}E} \propto e^{\beta E} \,. \tag{93}$$

In order to do this, let us notice that both terms in the upper bound of Eq. (91) are positive and must be simultaneously and independently small. For the first term, this trivially implies that $\|V\|_\infty \ll \varepsilon$. To find the condition for the second term, let us assume that the interaction does not shift excessively the energy levels such that $\Delta\Omega/\Omega_{\min}$ can be neglected. Thus,

$$1 \gg \frac{\Omega_\varepsilon}{2\,\Omega_{\min}} > \frac{\int_{E+\Delta-\varepsilon}^{E+\Delta} \varrho(E')\mathrm{d}E'}{2\int_E^{E+\Delta} \varrho(E')\mathrm{d}E'} = \frac{1-\mathrm{e}^{-\beta\varepsilon}}{2(1-\mathrm{e}^{-\beta\Delta})} \,, \tag{94}$$

and the condition $\beta\varepsilon \ll 1$ is required. These two necessary conditions can be summarized as

$$\beta\|V\|_\infty \ll \beta\varepsilon \ll 1 \,. \tag{95}$$

It is easy to see that they are also sufficient conditions by bounding Eq. (91),

$$\mathcal{D}(\omega_\sqcap^S, \omega_\sqcap^{S(0)}) \leq \frac{\|V\|_\infty}{\varepsilon} + \frac{\beta\varepsilon}{1-\mathrm{e}^{-\beta\Delta}} \,, \tag{96}$$

where it has been used that

$$\frac{\Omega_\varepsilon}{2\,\Omega_{\min}} < \frac{\int_{E+\Delta-\varepsilon}^{E+\Delta} \varrho(E')\mathrm{d}E'}{\int_E^{E+\Delta} \varrho(E')\mathrm{d}E'} = \frac{1-\mathrm{e}^{-\beta\varepsilon}}{1-\mathrm{e}^{-\beta\Delta}} \leq \frac{\beta\varepsilon}{1-\mathrm{e}^{-\beta\Delta}} \,.$$

Finally, let us simply choose $\varepsilon = \sqrt{\|V\|_\infty/\beta}$. The trace distance between the microcanonical states $\omega_\sqcap^{(0)}$ and $\omega_\sqcap$ then reads,

$$\mathcal{D}(\omega_\sqcap^S, \omega_\sqcap^{S(0)}) \leq \frac{2}{1-\mathrm{e}^{-\beta\Delta}} \sqrt{\beta\|V\|_\infty} \,. \tag{97}$$

Equation (97) ensures the indistinguishability of the interacting and non-interacting microcanonical states as long as $\Delta > k_B T$ is not too small and the condition

$$\|V\|_\infty \ll k_B T \,, \tag{98}$$

where k_B is the Boltzmann constant and T the absolute temperature, is fulfilled. That is, Eq. (97) gives us a physical intuition about when an interaction is weak in the sense of theorem 1. An interaction is weak if it is small with respect to the thermal energy, *i. e.* $k_B T$, which sets the intensive energy content of the system. This reflects the fact that how strong an interaction feels for the system depends on how much energy it contains.