The problem of equilibration and the computation of correlation functions on a quantum computer

Barbara M. Terhal and David P. DiVincenzo

1 ITF, Universiteit van Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, and CWI, Kruislaan 413, 1098 SJ Amsterdam, The Netherlands.

2 IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA.

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We address the question of how a quantum computer can be used to simulate experiments on quantum systems in thermal equilibrium. We present two approaches for the preparation of the equilibrium state on a quantum computer. For both approaches, we show that the output state of the algorithm, after long enough time, is the desired equilibrium. We present a numerical analysis of one of these approaches for small systems. We show how equilibrium (time)-correlation functions can be efficiently estimated on a quantum computer, given a preparation of the equilibrium state.

The quantum algorithms that we present are hard to simulate on a classical computer. This indicates that they could provide an exponential speedup over what can be achieved with a classical device.

I. THE LIMITS OF CLASSICAL COMPUTATION

The power of quantum computers has been demonstrated in several algorithms, of which the most striking have been Shor’s factoring algorithm and Grover’s search algorithm. From the very start however, the quantum computer has also held the promise of being a simulator of physical systems. This is the content of the physical version of the Church-Turing principle proposed by Deutsch. Thus we might expect that the universal quantum computer can be used to simulate any experiment that we could do on a real physical system. If such a simulation can be done efficiently (that is, without exponential slowdown), it is clear that this could be one of the major applications of a quantum computer. This promise seems to have been only partly fulfilled until now; it has been shown by several researchers that a simulation of the unitary time evolution of a physical system that possesses some degree of locality (which realistic physical systems do) can be accomplished efficiently on a quantum computer. However, many quantities of interest that are determined by experiment, or by the use of classical simulation techniques, relate to open quantum systems, in particular to systems in thermal equilibrium. The thermal equilibrium (Gibbs) state (in the canonical ensemble) of a Hamiltonian $H$ is given by

$$
\rho_\beta = \frac{1}{Z} \sum_{m=1}^{N} e^{-\beta E_m} |m\rangle \langle m|,
$$

where $|m\rangle$ ($E_m$) are the eigenvectors (eigenvalues) of $H$. $Z$ is the partition function

$$
Z = \sum_{m=1}^{N} e^{-\beta E_m},
$$

and $\beta = \frac{1}{kT}$ where $k$ is Boltzmann’s constant and $T$ the temperature. The physical systems that concern us in this paper will have a finite dimensional Hilbert space $\mathcal{H}$ that can be decomposed as

$$
\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \ldots \otimes \mathcal{H}_n,
$$

where each $\mathcal{H}_i$ represents a small, constant Hilbert space, typically associated with some (generalized) spin or other local degree of freedom. The Hamiltonian couples these local Hilbert spaces, for example in correspondence with a $d$-dimensional spatial lattice, so that there is only coupling between adjacent “spins” on this lattice. The quantities of interest, computed in experiment or in a classical computation, are of the form

$$
\text{Tr} \ O_1(t_1)O_2(t_2)O_3(t_3)\ldots O_k(t_k)\rho_\beta,
$$

where $O_i(t_i)$ are (possibly time-dependent) observables. Both for classical systems as well as for quantum systems, computational Monte Carlo methods have been developed to estimate correlation functions as in Eq. (1.4).
The quantum Monte Carlo method for systems at finite temperature relies on a transformation introduced by Suzuki \cite{10} that maps an initial quantum system on a \(d\)-dimensional lattice onto a \((d+1)\)-dimensional classical system. This conversion makes it possible to use classical computational sampling techniques to estimate correlation functions as in Eq. (1.4). There seem to be (at least) two situations when this approach runs into trouble and no good computational alternatives are available \cite{11}: (1) the correlation functions depend explicitly on time \(t\), and (2) the quantum system is of a fermionic nature. We will give a short explanation of why these problems are encountered.

The transformation from a classical to a quantum system is based on the generalized Trotter formula. Let \(H = \sum_{i=1}^{k} H_i\) where each \(H_i\) is a Hamiltonian on a small constant Hilbert space. The Trotter formula reads

\[
e^{\sigma H} = \lim_{n \to \infty} \left( e^{\sigma H_1/n} e^{\sigma H_2/n} \ldots e^{\sigma H_k/n} \right)^n.
\] (1.5)

The partition function Eq. (1.2) (and similarly correlation functions as in Eq. (1.4)) can be rewritten, using the Trotter formula and the identity \(\sum_m |a^m_{i,j}a^{m'*}_{i,j}| = 1\), where the pair of indices \((i,j)\) labels a choice of basis, as

\[
Z = \text{Tr} e^{-\beta H} = \sum_{\{a_{i,j}\}} p(a_{i,j}).
\] (1.6)

where \(p(a_{i,j})\) is a distribution over the values of the collection of variables \(\{a_{i,j}\}\) and \(j\) indexes the repetitions of the factors of Eq. (1.5) from 1 to \(n\). If the distribution is nonnegative, we can write \(p(a_{i,j}) = e^{H_{eff}(\{a_{i,j}\})}\) where \(H_{eff}\) is now a classical Hamiltonian given by

\[
H_{eff}(\{a_{i,j}\}) = \lim_{n \to \infty} \sum_{j=1}^{n} \sum_{i=1}^{k} \tilde{H}_i(a_{i,j}, a_{i+1,j}),
\] (1.7)

with \(a_{k+1,j} = a_{1,j+1}\), \(a_{k+1,n} = a_{1,1}\) and

\[
\tilde{H}_i(a, b) = \log(\langle a | \exp(-\beta H_i/n) | b \rangle).
\] (1.8)

The distribution \(p(a_{i,j})\) will only be nonnegative when the matrix elements \(\langle a | \exp(-\beta H_i/n) | b \rangle\) are positive. Thus it is important to choose the right sets of basis states \(|a^m_{i,j}\rangle\) to make the conversion to a classical sampling problem with a positive distribution. There are fermionic systems such as certain Hubbard models \cite{10} in which it does not seem to be possible to choose such a good basis. For these systems it has turned out to be very hard to get good estimates of correlation functions by using classical Monte Carlo techniques. This problem is usually referred to as the “sign” problem.

When we are to compute time-dependent quantities, for example the function \(f(it) = \text{Tr} e^{iHt} e^{-iHt} |O_1 e^{-iHt} O_2 \rho_\beta\) we need to use an imaginary time \(\tau = it\) to perform the conversion of Eq. (1.3) to a classical system (we expand \(e^{iHt}\) with the Trotter formula). From the classical Monte Carlo sampling of the function \(f(\tau)\) for real \(\tau\), we estimate \(\hat{f}(\tau)\) and then we could in principle analytically continue this function. However, we only have a finite number of samples of the function and each sample point has some inaccuracy. The errors that are introduced in estimating the Fourier components \(\hat{f}(\omega)\) from this data give rise to large fluctuations when we reconstruct \(f(it)\) with the Laplace transform

\[
f(it) = \int_{-\infty}^{\infty} d\omega e^{-\omega t} \hat{f}(\omega),
\] (1.9)

resulting in a bad approximation for the time correlation function \(f(it)\).

The relevance of estimating a simple time correlation function (an example of Eq. (1.4)) such as

\[
\text{Tr} [A(t), B(t')|\rho_\beta = \langle A(t), B(t')|s]\] (1.10)

where \(A\) and \(B\) are some Hermitian Heisenberg operators of the system, cannot be overestimated. Let us recall the many contexts in which Eq. (1.10) is used in describing experimental properties of many-particle quantum systems \cite{11}.

When \(A = B = u\), where \(u\) is the displacement field of a crystal, (1.10) describes the phonon dynamics of solids as probed by inelastic neutron scattering. When \(A\) and \(B\) are the number-density operator, the dielectric susceptibility is represented; this correlation function describes a variety of other experiments, including x-ray photoemission and the so-called x-ray edge singularity. When we study the current-current response function, we obtain the electrical conductivity as described by the Kubo formula. (The density-density and current-current response functions are
intimately related via the continuity equation.) Spin-dependent quantities are also of interest: with the spin-spin correlation function, information is obtained about the magnetic susceptibility, and thus the magnon dynamics of ferromagnets and antiferromagnets, the Kondo effect, and the magnetic-dipole channel in neutron scattering. And finally, if $A$ and $B$ involve anomalous pair amplitudes which involve Fermion operators like $a_{\downarrow}(k) a_{\uparrow}(-k)$, the presence and dynamics of a superconducting phase can be probed.

In short, the dynamic pair correlation functions provide a window on many of the interesting quantities in experimental physics, and it would be highly desirable to have a method of obtaining estimates for these quantities by simulation on a quantum computer. We will present some methods below for doing this.

In this paper we develop an approach to tackle these problems on a quantum computer. We break the problem into two parts: First, we present an approach to prepare our quantum computer in the equilibrium state $\rho_\beta$ of a given Hamiltonian (sections I and III). We will give two alternative routes to prepare an equilibrium state. Next we describe a procedure for efficiently estimating quantities as in Eq. (1.4) given that the equilibrium state has been prepared (section IV). We will not attempt to prove that our algorithms run in polynomial time even for a certain class of quantum systems $H$ and/or for certain ranges of $\beta$. The equilibration problem, in its full generality, is expected to be a hard problem. Even classically there is a large class of systems that exhibit a feature called frustration, for which calculating the partition function $Z$ as in Eq. (1.2) is a $P^c$-complete problem [12]. Also, for these systems, deciding whether the energy of the ground state is lower than some constant $K$ is an NP-complete problem [13]. The quantum problem has an added difficulty: We cannot assume that we know the eigenvectors (and eigenvalues) of the Hamiltonian of the system that we would like to equilibrate. There has been no demonstration yet that a quantum computer can exponentially outperform a classical computer in estimating the partition function for certain classical systems, which would enable us to sample efficiently from the classical Gibbs distribution [14].

The quantum algorithms that we present are hard to simulate on a classical computer. In both of our equilibration algorithms we use the fact that one can implement the unitary time evolution of a local Hamiltonian on systems, which would enable us to sample efficiently from the classical Gibbs distribution [14].

The quantum algorithms that we present are hard to simulate on a classical computer. In both of our equilibration algorithms we use the fact that one can implement the unitary time evolution of a local Hamiltonian on $n$ qubits in a polynomial number of steps in $n$ on a quantum computer [5]. A direct simulation of this procedure on a classical computer would cost exponential (in $n$) space and time and is therefore unrealistic. As we will show in section IV, given a preparation of an equilibrium state, there exists an efficient procedure on a quantum computer to calculate (time-dependent) correlation functions. As we discussed above, there is no general efficient classical algorithm with which one can estimate time-dependent correlation functions. Our quantum algorithm provides such an algorithm for a quantum computer. Lloyd and Abrams [16] have shown that the unitary simulation of a fermionic system such as the Hubbard model, either in first or second quantization, can be performed efficiently on a quantum computer. The quantum algorithms that we will present will use this unitary evolution as a building block. Therefore these algorithms can be used to compute correlation functions for the Hubbard model on a quantum computer. This is a task for which we do not have a good classical algorithm, due to the “sign” problem, as we pointed out above.

We focus our efforts on quantum equilibration algorithms for Hamiltonians of which the eigenvalues and eigenvectors are not known beforehand. These are the Hamiltonians of, for example, Heisenberg models (in more than two dimensions), Hubbard models, t-J models, XY models, or many-electron Hamiltonians in quantum chemistry. On the other hand, knowing the eigenvectors and eigenvalues of a Hamiltonian, such as in the Ising model, is no guarantee that there exists an efficient (polynomial time) classical algorithm that produces the equilibrium distribution. The situation is similar for quantum algorithms; we do not know in what cases the equilibration algorithms presented in section I and III give rise to a polynomial time algorithm (see also [15] for quantum algorithms for Ising-type models).

The process of equilibration is also essential in the actual realization of a quantum computer. One of the assumptions underlying the construction of a quantum computer [17] is the ability to put a physical system initially into a known state (or a thermal equilibrium state in the NMR quantum computer [18]), the computational $|00\ldots0\rangle/\langle00\ldots0|$ state. The way this is done in an experimental setup is to let this state be the ground state of a natural Hamiltonian and subsequently to cool to low temperature such that the probability of being in this ground state is some constant. This natural Hamiltonian must be sufficiently simple for this equilibration to be achievable efficiently and also be sufficiently weak or tunable not to disturb the computation later on.

II. EQUILIBRATION I

A. Introduction

The canonical ensemble is the ensemble of states $\{p_i, |\psi_i\rangle\}$, or a density matrix $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, such that $\rho$ has a given energy-expectation value

$$\text{Tr} \ H \rho = \langle E \rangle. \quad (2.1)$$

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The equilibrium state in this ensemble (Eq. (1.1)) can be obtained by maximizing the von Neumann entropy of $\rho$ under this energy constraint. Another way in which the canonical ensemble is defined is by considering the possible states of a system that is in contact with an infinite heat bath at a certain temperature $T$. The total energy of system and bath is constant, but bath and system exchange energy, so that the system equilibrates. This directly suggests that the way to prepare the equilibrium state on a quantum computer is to mimic this process. In considering the computational complexity of such a procedure, we will have to include the space and time cost of the bath, which may be large. Also, the intuitive picture of equilibration between a weakly coupled large bath and system does not tell us anything about the rate at which this equilibration occurs. Furthermore, the equilibration process assumes a bath that is already in its equilibrium state. Can we make the bath simple enough that this bath state can be prepared efficiently? In this section we study this process of equilibration. We present an algorithm and we derive expressions that completely characterize the equilibration process in an idealized case: the coupling between the bath and the system is very small, the bath is very large, and the time of interaction is large. We then proceed by a numerical study of the algorithm in realistic cases where the bath is of finite dimension, the strength of the interaction is non-zero, and the interaction time is limited.

B. The algorithm

**Definition 1 Equilibration algorithm I.**

**Input-parameters:**
- $H_s$, the Hamiltonian of a $N = 2^n$-dimensional quantum system.
- $\beta$, the inverse temperature.
- $H_b$, the Hamiltonian of a $K = 2^k$-dimensional “bath” quantum system.
- $\lambda H_{sb}$, where $H_{sb}$ is the $NK$-dimensional “bath-system” interaction Hamiltonian and $\lambda$ is the parameter that measures the strength of the interaction between bath and system.
- $t$, the interaction time between bath and system.
- $r$, the number of times the bath is refreshed in the algorithm.

Define the total Hamiltonian of system and bath as

$$H = H_s \otimes 1_K + 1_N \otimes H_b + \lambda H_{sb},$$

(2.2)

and the trace-preserving completely positive (TCP) map $S_{\lambda,t}$ as

$$S_{\lambda,t}(\rho) \equiv \text{Tr}_b e^{iHt} \rho \otimes \rho_{b,\beta} e^{-iHt}.$$  

(2.3)

1. **Prepare system.** We prepare the $n$ qubits in the computational 0 state: $|00\ldots00\rangle|00\ldots00\rangle$.

2. **Prepare bath.** We prepare the $k$ qubits of the bath in their equilibrium state $\rho_{b,\beta}$ of $H_b$.

3. **Evolve** system and bath for time $t$ and discard bath, that is, perform the superoperator $S_{\lambda,t}$ of Eq. (2.3).

4. **Repeat** steps 2 and 3 $r$ times such that

$$\|S_{\lambda,t}^{r+1}(|00\ldots00\rangle|00\ldots00\rangle) - S_{\lambda,t}^r(|00\ldots00\rangle|00\ldots00\rangle)\|_{tr} \leq \epsilon,$$

(2.4)

for all $r \geq r_0$ and $\epsilon$ is some accuracy. See Appendix [A] for the definition of $\| \cdot \|_{tr}$.

We put several constraints on $H_s, H_b$, and $H_{sb}$. We will use local Hilbert spaces as in Eq. (1.3) of dimension 2 (qubits). $H_s$ must be a “local” Hamiltonian. We define a $c$-local Hamiltonian on $n$ qubits as one that can be expressed as

$$H_s = \sum_{i=1}^{\text{poly}(n)} 1_{N/c} \otimes h_i,$$

(2.5)

where each $h_i$ operates on a tensor product of several small qubit Hilbert spaces, whose total dimension is $c$. We will also assume that the eigenvalues of $H_s$ are all distinct; the spectrum is non-degenerate. This will simplify the upcoming analysis. In order to treat Hamiltonians with degenerate spectra a change in the perturbation theory of Section II D will have to be made. We expect however that with that change the main result of Section II E, namely successful equilibration in the idealized case, will still hold. $H_{sb}$ has the linear coupling form.
\[ H_{sb} = S \otimes B, \]  
(2.6)

where both \( S \in B(H_s) \) and \( B \in B(H_b) \) are local Hamiltonians. \( H_b \) is the Hamiltonian of a system of non-interacting qubits, i.e., it is a sum of single-qubit Hamiltonians:

\[ H_b = \sum_{i=1}^{k} 1_{K/2} \otimes h_i. \]  
(2.7)

The bath's equilibrium state factorizes into a tensor product of qubit equilibrium states associated with each \( h_i \):

\[ \rho_{b,\beta} = \rho_{b,\beta}^0 \otimes \ldots \otimes \rho_{b,\beta}^k. \]  
(2.8)

This enables us to prepare the bath (step 2) efficiently. Appendix B shows that it will cost \( 2k \) elementary qubit operations to perform step 2. The locality of \( H_s \), \( H_b \), and \( H_{sb} \) is required in order to be able to simulate the unitary time evolution \( e^{iHt} \) in time proportional to \( t^2/\delta \) where \( \delta \) is the accuracy with which gates are implemented [5,19].

We also choose

\[ \langle B \rangle_b \equiv \text{Tr} \rho_{b,\beta} = 0. \]  
(2.9)

To understand the effect of a non-zero \( \langle B \rangle_b \) we rewrite \( H \) as

\[ H = (H_s + \lambda \langle B \rangle_b) S \otimes 1_K + 1_N \otimes H_b + \lambda S \otimes B', \]  
(2.10)

where \( \langle B \rangle_b = 0 \). Thus choosing a non-zero \( \langle B \rangle_b \) effectively corresponds to a change in the Hamiltonian of the system. We now discuss the last step of the algorithm, step 4. When the superoperator \( S_{\lambda,t} \) has the equilibrium state \( \rho_{s,\beta} \) as its unique fixed point, then Eq. (2.3) for all \( r \geq r_0 \) implies that that

\[ \| S_{\lambda,t}^r (|00\ldots00\rangle \langle 00\ldots00|) - \rho_{s,\beta} \|_{tr} \leq \epsilon. \]  
(2.11)

for all \( r \geq r_0 \), that is, the equilibration process leads to successful convergence to the equilibrium state. There does however not exist a straightforward implementation of step 4. The first problem is that we would have to check the closeness of the \( r \)th and the \((r+1)\)th iteration of \( S_{\lambda,t} \) for all \( r \geq r_0 \). In practice this has to be replaced with choosing a finite set of iterations \( r \) for which the invariance of \( S'(|00\ldots00\rangle \langle 00\ldots00|) \) is tested. This problem is also encountered in classical Monte Carlo simulations. The second problem, which is a purely quantum phenomenon, is that by measuring \( \rho_r \equiv S_{\lambda,t}^r (\rho) \) we might disturb \( \rho_r \). Thus to compare \( \rho_r \) with \( \rho_{r+1} \) we would have to run \( S \) again for \( r+1 \) times. To assemble some statistics on the difference between \( \rho_r \) and \( \rho_{r+1} \) we have to run \( r \) iterations of \( S \) several times. These considerations about the verification of the convergence of the equilibration process are of course not special to the use of a quantum computer; they are the same as in the equilibration of a quantum physical system in an experimental setup. Furthermore, it would be an impractical task to try to measure all the matrix elements of \( \rho_r \); \( \rho_r \) contains an exponential amount of data of which we can extract only a polynomial amount by measurement in polynomial time. The best way to proceed is the same as what one does in classical Monte Carlo simulations [3]. If the goal of the computation is to estimate \( \text{Tr} O \rho_{s,\beta} \) then one assembles the datapoints

\[ O_r = \text{Tr} O \rho_r, \]  
(2.12)

until \( |O_r - O_{r+1}| \leq \epsilon \) for a sufficiently large set of iterations \( r \geq r_0 \). The same procedure can be carried out when the goal of the equilibration is to compute a time-dependent correlation function such as Eq. (1.4).

In the remainder of this section we will analyse this algorithm. In section II D we discuss the non-hermitian perturbation theory that will be the basis of the analysis of \( S_{\lambda,t} \) in the idealized case. In section II E we derive explicit expressions for the idealized case. The idealized case is the case obtained by taking the limits \( \lambda \to 0 \), \( k \to \infty \) and \( t \to \infty \). We develop a perturbation theory on the basis of the assumption that \( S_{\lambda,t} \) of Eq. (2.3) is diagonalizable. Then we can show that in this idealized case the process has a unique fixed point which is the equilibrium state. Finally, in sections II F and II H we present results from numerical simulations in realistic cases. The following questions will be addressed:

1. How does \( k \), the number of bath qubits depend on \( n \), the number of system qubits? Are they polynomially related?
2. What is the influence of different choices for \( H_b \), \( S \) and \( B \) (Eqs. (2.6), (2.7))? 
3. How do the \( r \), \( \lambda \), and \( t \) required for successful equilibration depend on \( n \) generically?

The dynamics of open quantum systems, like the system in our algorithm that interacts with a bath, are most often studied with the use of a generalized master equation (21). The exact master equation in integral form describes the time evolution of \( \rho(t) = S_{\lambda,t}(\rho) \) of Eq. (2.3):
\[ \rho(t) = e^{-iL_s t} \rho(0) - \lambda^2 \int_0^t dt' \int_0^{t'} dt'' e^{-iL_s(t-t'')} \mathcal{M}(t', t'') \rho(t''). \]  

(2.13)

where \( L \), the Liouvillian, is defined as

\[ L(\rho) = [H, \rho], \]  

(2.14)

so that \( L_s(\rho) = [H_s, \rho] \) etc. The operator \( \mathcal{M}(t', t'') \) is the “memory kernel”,

\[ \mathcal{M}(t', t'') = \text{Tr}_b \left( e^{-i(1-p_\alpha) L_s} L(t'-t'') \right) L_{ab} \rho_b. \]  

(2.15)

The form in which the master equation is most often used, however, is one in which two simplifying approximations are made: (1) the Born approximation. This relates to the weakness of the interaction parameter \( \lambda \). (2) the Markov approximation. The process described by \( S_{\lambda,t} \) is Markovian if we can write

\[ S_{\lambda,t}(S_{\lambda,s}(\rho)) = S_{\lambda,t+s}(\rho). \]  

(2.16)

This typically occurs when the rate at which the effect of the system on the bath is erased in the bath (in the sense of being spread throughout the bath) is much faster than the rate at which the system evolves; the system sees a “fresh” bath every time. In our algorithm this loss of correlations in the bath is enforced when after some time \( t \) the bath is replaced by a new bath (step 4). We would not be able to truly equilibrate a finite system with a finite-dimensional bath if we would not keep refreshing it. Since the global evolution of bath and system is unitary, eventually we will get back to the initial unentangled state and, after tracing over the bath, to the initial state of the system (a so-called Poincaré recurrence). Whether Markovian dynamics is justified will depend on the size of the bath, the strength of the interaction and the length of the interaction time. There are ways to make a simple but naive Markov approximation in Eq. 2.13 that lead to a master equation that fails to describe TCP dynamics \[21, 22\]. The form of the master equation that does incorporate both the approximations and yields a physical completely positive map is the master equation in Lindblad form \[22\]:

\[ \frac{\partial \rho}{\partial t} = -i[H_s, \rho(t)] + L(\rho) \]  

(2.17)

where \( L \) \[24, 22\] can be expressed with a basis of operators \( F_i \) as

\[ L(\rho(t)) = \frac{1}{2} \sum_{k,l=1}^{N^2-1} a_{kl}([F_k \rho(t), F_l^\dagger] + [F_k, \rho(t) F_l^\dagger]), \]  

(2.18)

where \( a_{kl} \) is a positive semi-definite matrix. In a Lindblad equation describing the equilibration process, we expect \( L \) to depend on the system Hamiltonian \( H_s \). The equilibrium state \( \rho_{s,\beta} \) if the algorithm is successful– should be a stationary state of the process, which implies that \([H_s, \rho_{s,\beta}] = 0\) and

\[ L(\rho_{s,\beta}) = 0. \]  

(2.19)

Davies \[24, 26\] has demonstrated that a process described by \( S_{\lambda,t} \) where the bath is an infinite-dimensional quantum system (for example a quantum field) does equilibrate any quantum system in the limit where \( \lambda \to 0, t \to \infty \), but \( \lambda^2 t \) stays constant. By carefully taking a Born and Markov approximation, he derives a Lindblad equation of the form such that Eq. 2.19 is obeyed. We will perform a similar analysis here. The main point of difference is that we use a perturbative analysis of the dynamics which is only valid for small \( \lambda^2 t \), but coincides in this regime with Davies’ result. We furthermore obtain more explicit expressions for the dynamics in this limit.

One can write the most general form of an \( L \) that obeys a quantum detailed balance \[27\] condition, a stronger requirement that the stationarity of Eq. 2.19. Now, one might ask the following question: Could we implement this corresponding superoperator directly, without the use of a weakly coupled large bath, so as to save us time and space? We believe the answer is no, as \( L \) will depend on the eigenvectors and eigenvalues of \( H_s \), which we do not know beforehand.

### C. Some useful properties of TCP maps

In this section, we study some essential properties of the superoperator \( S_{\lambda,t} \) defined as in Eq. 2.3. This superoperator is a TCP map
where $B$ is the algebra of bounded operators on the Hilbert space $\mathcal{H}_N$. The set TCP$[N,N]$ is the set of TCP maps $S: B(\mathcal{H}_N) \to B(\mathcal{H}_N)$.

The elements of $B(\mathcal{H}_N)$ can be represented as $N \times N$ matrices. An alternative and convenient way to represent $B(\mathcal{H}_N)$ is as a $N^2$-dimensional complex vector space $\mathbb{C}^{N^2}$

\[ I: \chi \in B(\mathcal{H}_N) \to (\chi)_{ij} \in \mathbb{C}^{N^2}. \tag{2.21} \]

This representation leads to a matrix representation of a TCP map $S$ on $\mathbb{C}^{N^2}$. Let $A_i$ be the operation elements of $S$, i.e.

\[ S(\chi) = \sum_i A_i \chi A_i^\dagger, \quad \sum_i A_i^\dagger A_i = 1_N. \tag{2.22} \]

Then

\[ \chi'_{mn} = (S(\chi))_{mn} = \sum_i \sum_{k,l} (A_i)_{mk}(\chi)_{kl}(A_i^\dagger)_{ln} = \sum_i S_{mn,kl}(\chi)_{kl}, \tag{2.23} \]

with

\[ S_{mn,kl} = \sum_i (A_i)_{mk}(A_i^\dagger)_{ln}. \tag{2.24} \]

One can then study the eigenvectors and eigenvalues of the matrix representation of a TCP map. First, we will give three useful properties of TCP maps that follow directly from their definition:

**Property 1** Let $B_{pos} \in B$ be the set of positive semi-definite matrices. Let $S \in TCP[N,N]$. Then

\[ \rho \in B_{pos} \Rightarrow S(\rho) \in B_{pos}, \tag{2.25} \]

as $S$ is (completely) positive. Let $\chi$ be an eigenvector of $S$ with eigenvalue $\mu$, $S(\chi) = \mu \chi$. We have

\[ Tr \chi \neq 0 \Rightarrow \mu = 1, \tag{2.26} \]

as $S$ is trace-preserving. Let $A_i$ be the operation elements in the decomposition of $S$ as in Eq. (2.22). If $\chi$ is an eigenvector of $S$ with eigenvalue $\mu$, then $\chi^\dagger$ is also an eigenvector of $S$ with eigenvalue $\mu^*$. This follows from

\[ (S(\chi))^\dagger = \sum_i (A_i \chi A_i^\dagger)^\dagger = S(\chi^\dagger). \tag{2.27} \]

Let $B_{pos,1}$ be the set of positive semi-definite matrices that have trace 1, i.e. the density matrices. Thus Property 1 implies that if a density matrix $\rho$ is an eigenvector of the superoperator, it must have eigenvalue 1, that is, it is a fixed point of the map. On the basis of the TCP property of a map $S$, we can also show the following:

**Proposition 1** Let $S \in TCP[N,N]$. All eigenvalues $\mu$ of $S$ have $|\mu| \leq 1$.

**Proof** (by contradiction): Assume $\chi$ is an eigenvector of $S$ with eigenvalue $|\mu| > 1$. Note that Property 1 implies that $\chi$ has $Tr \chi = 0$. If $\chi$ is hermitian, $\mu$ will be real. As $\chi$ is traceless, it must have at least one negative eigenvalue. One can always find a density matrix $\rho$ and a small enough $\epsilon$ such that $\rho' = \rho + \epsilon \chi$ is still a density matrix. Let $S$ operate $r$ times on this density matrix. For large enough $r$ the result $S^r(\rho + \epsilon \chi) = S^r(\rho) + \epsilon \mu^r \chi$ will no longer be a positive semi-definite matrix: take the eigenvector $|\psi\rangle$ of $\chi$ corresponding to the lowest (negative) eigenvalue $\lambda_{\text{min}}$. Then

\[ \langle \psi | S^r(\rho) | \psi \rangle + \epsilon \mu^r \langle \psi | \chi | \psi \rangle \leq 1 + \epsilon \mu^r \lambda_{\text{min}}, \tag{2.28} \]

will become negative for large enough $r$. But Property 1 implies that $S^r(\rho')$ is a density matrix, thus $|\mu|$ cannot be larger than 1. When $\chi$ is non-hermitian, we reason similarly. One can find a density matrix $\rho$ and a small enough $\epsilon$ such that $\rho' = \rho + \epsilon (\chi + \chi^\dagger)$ is a density matrix. Let $S(\chi) = \mu \chi = |\mu| e^{i\phi} \chi$. Let $\lambda_{\text{min},r}$ be the smallest (and negative) eigenvalue of the traceless hermitian matrix $e^{i\phi} \chi + e^{-i\phi} \chi^\dagger$. Then

\[ \langle \psi | S^r(\rho') | \psi \rangle = \langle \psi | S^r(\rho) | \psi \rangle + \epsilon |\mu|^r \langle \psi | (e^{i\phi} \chi + e^{-i\phi} \chi^\dagger) | \psi \rangle \leq 1 + \epsilon |\mu|^r \lambda_{\text{min},r}, \tag{2.29} \]

will become negative for some large $r$ ($\lambda_{\text{min},r}$ is a quasi-periodic function of $r$ so it cannot be small for all large $r$). □

Another property about the existence of fixed points can be derived:
Proposition 2 Let $S \in TCP[N, N]$. $S$ has a fixed point (which is a density matrix).

Proof: The set of density matrices $B_{pos, 1} \in B(H_N)$ is convex and compact. $S$ is a linear continuous map and $S(\rho \in B_{pos, 1}) \in B_{pos, 1}$. Then the Markov-Kakutani Theorem V.10.6 of [23] applies. □

The existence of a fixed point does not by itself guarantee that the process described by $S$ is “relaxing”, that is, $\lim_{r \to \infty} S^r(\rho) = \rho_0$ for all $\rho$ where $\rho_0$ is the fixed point. The existence of such a limit depends on whether the fixed point is unique. This following Proposition proves that when there is unique fixed point, relaxation will occur and the relaxation rate is determined by the second largest eigenvalue of $S$.

Proposition 3 Let $\rho_0 \in B_{pos, 1}(H_N)$ be the unique fixed point of a TCP map $S$. Let $|\kappa| = \max_{m \neq 0} |\mu_m|$, the absolute value of the second largest eigenvalue of $S$. Then for all density matrices $\rho$ we have

$$
\| S^r(\rho) - \rho_0 \|_{tr} \leq C_N \text{poly}(r)|\kappa|^r.
$$

(2.30)

where $C_N$ is a constant depending on the dimension $N$ of the system and poly$(r)$ denotes some polynomial in $r$. Thus for all density matrices $\rho$

$$
\lim_{r \to \infty} \| S^r(\rho) - \rho_0 \|_{tr} = 0.
$$

(2.31)

Proof: Let $\mu_i$ be the eigenvalues of $S$. Let $s$ be the number of distinct eigenvalues. We can bring any matrix $S$ into Jordan form $J$ by a similarity transformation $M$ [31]:

$$
S = MJM^{-1},
$$

(2.32)

where

$$
J = \sum_{i=1}^{s} (\mu_i P_i + N_i).
$$

(2.33)

$P_i$ are orthogonal projectors and $N_i$ is a matrix of 1s above the diagonal in the $i$th block or $N_i$ is the 0 matrix. When the eigenvalue $\mu_i$ is nondegenerate $N_i$ is the 0 matrix. We therefore have $N_i N_j = 0$ for $i \neq j$ and $P_i N_j = 0$ for $i \neq j$.

Call the unique largest eigenvalue $\mu_0 = 1$ and the corresponding projection $P_0$. As in Eq. (2.32) one can write

$$
S^r = MJ^rM^{-1}.
$$

(2.34)

where $J^r$ equals

$$
J^r = \sum_{i=1}^{s} (\mu_i^r P_i + N_i^r)
$$

(2.35)

where $N_i^r$ is a nilpotent matrix in the $i$th block whose matrix elements are all smaller than or equal to $r\mu_i^r$. Note that $N_0$ is not present as $\mu_0$ is unique. Let $S^0$ be $MP_0 M^{-1}$ or $S^0(\rho) = \rho_0$. We use $\|A\|_{tr} \leq \sqrt{N} \|A\|_2$. Note that $\|A\|_2$ refers to the Euclidean norm of $A$ represented as a vector. This follows from $(\sum_{i=1}^{N} |x_i|^2)^2 \leq N \sum_{i=1}^{N} |x_i|^2$ for complex numbers $x_i$. We have first of all

$$
\| S^r(\rho) - \rho_0 \|_{tr} \leq \sqrt{N} \| (S^r - S^0)(\rho) \|_2.
$$

(2.36)

This expression can be bounded with the use of the similarity transformation $M$ to

$$
\| S^r(\rho) - \rho_0 \|_{tr} \leq \sqrt{N} \| M(S^r - S^0)M^{-1} \|_2 \leq C_{1, N} \| J^r - P_0 \|_2
$$

(2.37)

where $\|\cdot\|_2$ is defined in Appendix A and we use $\|\rho\|_2 = \text{Tr} \rho^2 \leq 1$ for density matrices. Using the expression for $J^r$, Eq. (2.33), we can also bound

$$
\| J^r - P_0 \|_2 \leq \text{poly}(r)C_{2, N}|\kappa|^r.
$$

(2.38)

Combining Eq. (2.37) and Eq. (2.38) gives us the desired result Eq. (2.30). Eq. (2.31) then follows as $|\kappa| < 1$ by Proposition □. If $S$ is diagonalizable, the nilpotents $N_i$ in expression Eq. (2.33) are not present. By going through the same steps, a bound as in Eq. (2.30) can be derived without the factor poly$(r)$. □
We refer the reader to [22] for discussions and references concerning the existence of a unique fixed point and other properties of relaxation for a process that is described by a Lindblad equation, Eq. (2.17).

The bound on the rate of convergence of Eq. (2.30) is far from optimal for small $r$ as we know that for any two density matrices $\rho_1$ and $\rho_2$, $\|\rho_1 - \rho_2\|_{tr} \leq 2$. However, it is not so bad as to invalidate the main conclusion that one would like to draw from it. If $S$ is diagonalizable and $|\kappa| = 1 - a/n^c$ then a (polynomial) number of iterations $r = \frac{n^c}{a} (\ln 1/\epsilon + \ln C_N)$, for large $n$, results in

$$\| S^r (\rho) - \rho_0 \|_{tr} \leq \epsilon,$$

(2.39)

where we used $\lim_{m \to \infty} (1 - x/m)^m = e^{-x}$. If $S$ is not diagonalizable the convergence is possibly slowed by the factor $\text{poly}(r)$, but there still will be a polynomial relation between $|\kappa|$ and $r$.

Finally we give a result which relates members of TCP$[N,N]$ to the stochastic matrices. A real matrix $M$ is stochastic when the entries of its columns add up to 1, i.e.

$$\sum_i M_{ij} = 1.$$

Proposition 4 Let $S \in$ TCP$[N,N]$. $S_{mm,nn} \in \mathbb{R}$, and, $\forall n$, $\sum_m S_{mm,nn} = 1$; that is, the elements $S_{mm,nn}$ form an $N \times N$ stochastic matrix in the indices $m$ and $n$. Also, $\forall n,k$, $n \neq k$, $\sum_m S_{mm,nk} = 0$.

Proof: $S_{mm,nn} \in \mathbb{R}$ follows directly from Eq. (2.24). For the rest, we impose the unit trace condition on Eq. (2.23):

$$1 = \sum_{m,k,l} S_{mm,kl} \rho_{kl}.$$  

(2.40)

This must be true for all density matrices represented by $\rho$. Taking $\rho_{kl} = \delta_{k,l} \delta_{k,k_0}$ gives the desired result

$$1 = \sum_m S_{mm,k_0k_0}.$$  

(2.41)

We now separate Eq. (2.40) into diagonal and off-diagonal parts, using the Hermiticity of the density matrix $\rho$:

$$1 = \sum_{m,k,l} S_{mm,kl} \rho_{kl} + \sum_{m,k,l} (S_{mm,kl} + S_{mm,lk}) \text{Re}(\rho_{kl}) + i \sum_{m,k,l} (S_{mm,kl} - S_{mm,lk}) \text{Im}(\rho_{kl}).$$  

(2.42)

The first term of Eq. (2.42) is always 1 because of Eq. (2.41). If we require Eq. (2.42) when the off-diagonal terms in $\rho$ are $\rho_{kl} = \delta_{k,k_0} \delta_{l,l_0}$ ($k > l$), we obtain

$$\sum_m (S_{mm,k_0l_0} + S_{mm,l_0k_0}) = 0,$$

(2.43)

and setting the off-diagonal terms in $\rho$ to $\rho_{kl} = i\delta_{k,k_0} \delta_{l,l_0}$ ($k > l$) gives

$$\sum_m (S_{mm,k_0l_0} - S_{mm,l_0k_0}) = 0,$$

(2.44)

Adding these equations, we obtain the desired result

$$\sum_m S_{mm,k_0l_0} = 0, \quad k_0 \neq l_0.$$  

(2.45)

\[\square\]

D. Perturbation theory

In this section we develop a perturbation theory in the coupling $\lambda$ for the superoperator $S_{\lambda,t}$. The calculation will assume the diagonalizability of $S_{\lambda,t}$. If all the eigenvalues of a matrix $M$ are distinct, $M$ is diagonalizable [31]. Therefore in many cases of interest for equilibration, this assumption for $S_{\lambda,t}$ will be correct. An example of a simple superoperator that is nondiagonalizable is the following. The superoperator $S$ operates on $B(\mathcal{H}_3)$ and is given by
The eigenvectors of \( S \) are \( |i\rangle \langle j| \) for all \( i \neq j \), the state \( |2\rangle \langle 2| \) and \( |1\rangle \langle 1| - |2\rangle \langle 2| \). This example shows that non-diagonalizability is not a property particular to superoperators describing quantum operations but is also found in classical Markov processes.

One can formally expand the superoperator \( S_{\lambda,t} \) as a power series in the coupling parameter \( \lambda \),

\[
S_{\lambda,t} = S_t^{(0)} + \lambda S_t^{(1)} + \lambda^2 S_t^{(2)} + \lambda^3 S_t^{(3)} + \ldots .
\]  

(2.47)

In section II E we will explicitly calculate the expressions for these expansion operators. We will show (Eqs. (2.70)-(2.73)) that condition Eq. (2.9) implies that \( S_t^{(1)} \) is zero for all \( t \). On the basis of this expansion, we will make a perturbative expansion of the eigenvalues and eigenvectors of \( S_{\lambda,t} \)

\[
\mu = \mu^{(0)} + \lambda \mu^{(1)} + \lambda^2 \mu^{(2)} + \ldots ,
\]

(2.48)

\[
\chi = \chi^{(0)} + \lambda \chi^{(1)} + \lambda^2 \chi^{(2)} + \ldots .
\]

(2.49)

Assuming that the perturbation expansion exists for this non-Hermitian operator, it will have the same structure as in the well established procedures familiar in quantum theory for bounded Hermitian operators (see textbooks on quantum mechanics such as [30] or [31] for a more mathematical background).

In the representation of Eq. (2.24) \( S_t^{(0)} \) reads

\[
(S_t^{(0)})_{mn,kl} = (U^t)_{mk}(U^{t \dagger})_{ln},
\]

(2.50)

where \( U = e^{iHs} \). Unitarity of \( S_t^{(0)} \), as a matrix operator on \( \mathbb{C}^{N^2} \), follows from

\[
\sum_{k,l} (S_t^{(0)})_{mn,kl}(S_t^{(0) \dagger})_{kl,ij} = \sum_{k,l} (U^t)_{mk}(U^{t \dagger})_{ln}(U^t)_{ji}(U^{t \dagger})_{ki} = \delta_{ml}\delta_{jn}.
\]

(2.51)

The eigenbasis of \( S_t^{(0)} \) is formed by the set of matrices \( \rho_{nm} \equiv |n\rangle \langle m| \) where \( |n\rangle \) are the eigenvectors of \( H_s \). These eigenvectors come with eigenvalues \( \mu^{(0)}_{t,nn} \):

\[
\{ \rho_{nm}, \mu^{(0)}_{t,nm} = e^{it(E_n - E_m)} \}_{n,m=1}^{N,N},
\]

(2.52)

where \( E_n \) are the eigenvalues of \( H_s \). Thus all density matrices of the form \( \rho_{nm} \), and mixtures of these, have degenerate eigenvalues \( \mu^{(0)}_{t,nn} = 1 \). If the spectrum of \( H_s \) is non-degenerate (we assumed this in section II B), then all other eigenvectors \( \rho_{nm} \) for \( n \neq m \) have non-degenerate eigenvalues. These eigenvectors \( \rho_{nm} \) form an orthonormal set with the vector inner product on \( \mathbb{C}^{N^2} \),

\[
\text{Tr} \rho_{nm}^{\dagger} \rho_{kl} = \delta_{nk}\delta_{ml}.
\]

(2.53)

To carry out the perturbation theory, we switch to a ket notation for the density operators and a matrix notation for the superoperators. This will make it easier for us to perform the necessary manipulations of degenerate perturbation theory, in which the degenerate sector is isolated and a diagonalization performed within it.

We first organize the diagonal, degenerate part of this vector space to be indexed. To be specific, we introduce an orthogonal basis in this vector space such that

\[
|\phi^{(0)}_i\rangle = \rho_{ii}, \quad 1 \leq i \leq N,
\]

(2.54)

\[
|\phi^{(0)}_{i(m,n)}\rangle = \rho_{mn}, \quad 1 \leq m,n \leq N, \quad m \neq n.
\]

(2.55)

In the second equation the indexing \( i \) can be made consecutive by choosing

\[
i(m,n) = nN + m - \frac{1}{2}n(n + 1), \quad m > n,
\]

\[
i(m,n) = \frac{1}{2}N(N - 1) + mN + n - \frac{1}{2}m(m + 1), \quad n > m.
\]

(2.56)
This organizes this new vector space into a direct-sum form $C^{N^2} = C_D \oplus C_{ND}$, where “$D$” and “$ND$” stand for diagonal and nondiagonal (or, degenerate and nondegenerate). $C_D$ has dimension $N$ and $C_{ND}$ has dimension $N^2 - N$.

From the discussion above, we note that the degeneracy is lifted in lowest order by the second-order part of the superoperator $S$ in the $D$ sector, which we will denote $S^{(2)}_{D,D}$. Assume that $S^{(2)}_{D,D}$ is diagonalizable via the similarity transformation

$$MS^{(2)}_{D,D}M^{-1} = \tilde{S}^{(2)}_{D,D},$$

where $\tilde{S}^{(2)}_{D,D}$ is a diagonal matrix (the tilde will denote quantities expressed in the new basis $M_D \oplus 1_{ND}|\phi^{(0)}\rangle$, which is in general non-orthogonal). In this new basis, the degeneracy of the diagonal terms of $S$ is lifted to second order in $\lambda$ (the diagonal terms can be written to second order as $\mu_i = 1 + \lambda^2 \tilde{S}^{(2)}_{ii}$, and since the largest off-diagonal terms in the $D$ sector are now third order, given by

$$\lambda^3 MS^{(3)}_{D,D}M^{-1} = \lambda^3 \tilde{S}^{(3)}_{D,D},$$

the condition for the successful application of non-degenerate perturbation theory is now satisfied, assuming that no additional, accidental degeneracy occurs. (The condition is satisfied from the start in the $ND$ sector.) Its form is essentially no different from the conventional perturbation expansion \cite{30} for Hermitian operators. This expansion for the eigenvalues is

$$\mu_i = \mu^{(0)}_i + \lambda^2 \tilde{S}^{(2)}_{ii} + O(\lambda^3).$$

The form of this expansion is different depending on whether $i \in D$ or $i \in ND$, but only at $O(\lambda^4)$. The perturbation expansions for the eigenvectors are

$$|\phi_i\rangle = |\phi^{(0)}_i\rangle + \lambda \sum_{j \in D, j \neq i} |\phi^{(0)}_j\rangle \frac{\tilde{S}^{(3)}_{ji}}{\tilde{S}^{(2)}_{ii} - \tilde{S}^{(2)}_{jj}} + O(\lambda^2), \quad i \in D,$$

$$|\phi_i\rangle = |\phi^{(0)}_i\rangle + \lambda^2 \sum_{j \neq i} |\phi^{(0)}_j\rangle \frac{\tilde{S}^{(2)}_{ji}}{\mu^{(0)}_i - \mu^{(0)}_j} + O(\lambda^3), \quad i \in ND.$$

This expansion indicates that there is no mixing between the $D$ and $ND$ sectors until second order in $\lambda$. This expansion strategy will be taken up again in the numerical simulations, Sec. II G (Eq. (2.116)).

We note that this separation of the superoperator into $D$ and $ND$ sectors permits us to write the action of the superoperator Eq. (2.47) using a more informative expression in which these sectors are almost decoupled:

$$(S_{\lambda,t}(\rho))_{nn} = \sum_m P_{nm,t} \rho_{mm} + \delta \rho_{nn},$$

$$P_{nm,t} = \delta_{nm} + \lambda^2 (S^{(2)}_{t})_{nn,mm} + \lambda^3 (S^{(3)}_{t})_{nn,mm} + \ldots,$$

$$\rho_{nn} = \lambda^2 \sum_{k,l,k \neq l} (S^{(2)}_{t})_{nn,kl} \rho_{kl} + \lambda^3 \sum_{k,l,k \neq l} (S^{(3)}_{t})_{nn,kl} \rho_{kl} + \ldots.$$ (2.64)

Note from Proposition 3 that $P_{nm,t}$ is exactly a stochastic matrix; therefore the dynamics in the $D$ sector is that of a classical Markov process, up to second order in $\lambda$ (since the contribution from the $ND$ sector, Eq. (2.64), is $O(\lambda^2)$). The dynamics inside the $ND$ sector is also simple:

$$(S_{\lambda,t}(\rho))_{nm} = \mu^{(0)}_{t,nn} \rho_{nm} + \lambda^2 \sum_{k,l,k \neq l} (S^{(2)}_{t})_{nm,kl} \rho_{kl} + \ldots, \quad n \neq m.$$ (2.65)

So, to $O(\lambda^2)$, there are no contributions to this equation from the $D$ sector. So, the low-order dynamics in the $ND$ sector simply involves a scalar multiplication of the off-diagonal components of the input matrix $\rho$.

The simplifications of Eqs. (2.62) and (2.63) makes it possible to answer questions about the uniqueness of the fixed point and, in principle, the mixing properties of a repeated application of $S_{\lambda,t}$, using techniques from classical Markov processes \cite{32}. The splitting in two sectors, each having its own relaxation times, is similar to the phenomenological
Then the condition Eq. (2.9) implies that $S$ of the trace and $H$ invariant under unitary evolution with $e^{-iHt}$, where $S$ and the operators $S_{\lambda,t}$ to zeroth order in $\lambda$ and the eigenvalues to second order in $\lambda$. The stochastic matrix $P_{nm,t}$ is determined in this approximation. The justification of this approximation will be given when we explicitly determine the expressions for $S_{\lambda,t}$ in section II E, where we set bounds on $\lambda$ and $t$ such that indeed $\lambda^2$ and higher order corrections are small within some norm (for example the $\|\cdot\|_\infty$ given in [34, 35]).

### E. Calculation of expressions

Here we will calculate the elements of the superoperator described in the last section to lowest non-trivial order in $\lambda$ ($\lambda^2$). Truncating the expression for $P$ in Eq. (2.63) to second order, $Q_{nm,t}$ is defined by the expression

$$P_{nm,t} \approx \delta_{nm} + \lambda^2 Q_{nm,t}.$$  

(2.66)

And taking $\mu$ in Eqs. (2.65,2.64) to second order, and using Eq. (2.52), we define $\nu_{nm,t}$ by

$$\nu_{nm,t} \approx e^{i(E_n - E_m)} (1 + \lambda^2 \nu_{nm,t}).$$  

(2.67)

In this section we will find expressions for $Q_{nm,t}$ and $\nu_{nm,t}$ and exhibit the regime in which they give a valid description of $S_{\lambda,t}$. We also show that for a large enough bath, the equilibrium state is the fixed point of the map $S_{\lambda,t}$. We discuss under what conditions this fixed point is unique.

We will use operators in the Heisenberg representation. We denote such operators (for example on the system) as

$$A_t = e^{iH_s t} A e^{-iH_s t}.$$  

(2.68)

The total Liouvillian $\mathcal{L}$ is defined as

$$e^{-i\mathcal{L}t}(\rho \otimes \rho_{b,\beta}) = U_t (\rho \otimes \rho_{b,\beta}) U_t^\dagger.$$  

(2.69)

One can expand the operator $e^{-i\mathcal{L}t}$ in a perturbation series in $\lambda$ [20], take a partial trace over the bath and identify the operators $S_t^{(0)} = e^{-i\mathcal{L}_s t}$, $S_t^{(1)}$ and $S_t^{(2)}$ in Eq. (2.47):

$$S_t^{(1)} = -i \text{Tr}_b \int_0^t dt' e^{-i(\mathcal{L}_s + \mathcal{L}_b)(t-t')} \mathcal{L}_{sb} e^{-i(\mathcal{L}_s + \mathcal{L}_b)t'},$$  

(2.70)

and

$$S_t^{(2)} = -\text{Tr}_b \int_0^t dt' \int_0^{t'} dt'' e^{-i(\mathcal{L}_s + \mathcal{L}_b)(t-t')} \mathcal{L}_{sb} e^{-i(\mathcal{L}_s + \mathcal{L}_b)(t'-t'')} \mathcal{L}_{sb} e^{-i(\mathcal{L}_s + \mathcal{L}_b)t''}.$$  

(2.71)

First we consider $S_t^{(1)}$. We use Eq. (2.69) and Eq. (2.14) to rewrite $S_t^{(1)}$ acting on $\rho \otimes \rho_{b,\beta}$ as:

$$S_t^{(1)}(\rho \otimes \rho_{b,\beta}) = -i\lambda \text{Tr}_b \int_0^t dt' e^{iH_s(t-t')} \rho \otimes \rho_{b,\beta} (H_{sb} \rho_{b} \otimes \rho_{b,\beta} + H_{b} \rho_{b} \otimes \rho_{b,\beta} + H_{b} \rho_{b} \otimes \rho_{b,\beta} + H_{b} \rho_{b} \otimes \rho_{b,\beta}) e^{-iH_s(t-t')} \rho \otimes \rho_{b,\beta},$$  

(2.72)

where $\rho_{b}$ is the time-evolved (with $H_s$) $\rho$ and $\rho_{b,\beta'}$ is the time-evolved (with $H_b$) $\rho_{b,\beta}$. The equilibrium state $\rho_{b,\beta}$ is invariant under unitary evolution with $e^{iH_s t'}$, and thus $\rho_{b,\beta'} = \rho_{b,\beta}$. We then use the cyclic permutation invariance of the trace and $H_{sb} = S \otimes B$ to rewrite equation (2.72) as a simpler sum of two terms

$$S_t^{(1)}(\rho \otimes \rho_{b,\beta}) = -i\lambda \int_0^t dt' \left[ e^{iH_s(t-t')} S \rho_{b} e^{-iH_s(t-t')} - e^{iH_s(t-t')} \rho_{b} e^{-iH_s(t-t')} \right] \text{Tr}_b B \rho_{b,\beta}$$  

(2.73)

Then the condition Eq. (2.9) implies that $S_t^{(1)}(\rho \otimes \rho_{b,\beta}) = 0$ for any $\rho$.

Let us consider the second order term. The expression for $S_t^{(2)}$ reads...
\[ S_t^{(2)} = -e^{-it\cdot t} \int_0^t dt' \int_0^{t'} dt'' \left( h(t' - t'')S_{-\nu}S_{-\nu} \rho - h(t'' - t')S_{-\nu} \rho S_{-\nu} \right) - h(t' - t'')S_{-\nu} \rho S_{-\nu} + h(t'' - t')\rho S_{-\nu}S_{-\nu}, \]

(2.74)

where \( h(t) \) is defined as \( \langle BB_t \rangle_b \). We write

\[ h(t) = \int_{-\infty}^{\infty} d\omega \; e^{i\omega t} \hat{h}(\omega). \]  

(2.75)

Let \( S_{nm} \) be the matrix elements of the interaction \( S \) in this eigenbasis of \( H_s \), \( S_{nm} = \langle n|S|m \rangle \). Now we can find the expression for \( Q_{mn,t} = \langle \hat{S}_t^{(2)} \rangle_{nm,nm} \). From Eq. (2.74) after integration over the variables \( t' \) and \( t'' \) and with the use of Eq. (2.72), we find:

\[ Q_{mn,t} = 2 \int_{-\infty}^{\infty} d\omega \; \hat{h}(\omega) \left[ |S_{mn}|^2 \left( 1 - \cos t(\omega - E_n + E_m) \right) \right] - \sum_l \frac{\delta_{nm} |S_{nl}|^2 (1 - \cos t(\omega - E_n + E_l))}{(\omega - E_n + E_l)^2}. \]  

(2.76)

For the “decay factor” \( \nu_{nm,t} \) in the ND sector we find

\[ \nu_{nm,t} = \int_{-\infty}^{\infty} d\omega \; \hat{h}(\omega) \left[ \frac{2S_{mn}S_{nm}(1 - \cos t\omega)}{\omega^2} - f(t, \omega, E_n) - f^*(t, \omega, E_m) \right], \]  

(2.77)

with \( f^* \) the complex conjugate of \( f \). The function \( f \) is given by

\[ \text{Re} \; f(t, \omega, E_n) = \sum_l \frac{|S_{ln}|^2 (1 - \cos t(\omega - E_n + E_l))}{(\omega - E_n + E_l)^2}, \]  

(2.78)

and

\[ \text{Im} \; f(t, \omega, E_n) = \sum_l \frac{|S_{ln}|^2}{\omega - E_n + E_l} \left[ 1 - \frac{\sin t(\omega - E_n + E_l)}{t(\omega - E_n + E_l)} \right]. \]  

(2.79)

We will now look at the idealized case, i.e., we take the limits (remember \( k \) is the number of qubits in the bath)

\[ P_{nm,\lambda^2 t} \equiv \lim_{t \to \infty, \lambda \to 0} \lim_{k \to \infty} P_{nm,t}, \quad \mu_{nm,\lambda^2 t} \equiv \lim_{t \to \infty, \lambda \to 0} \lim_{k \to \infty} (1 + \lambda^2 \nu_{nm,t}). \]  

(2.80)

When the bath is infinitely large, it will have a continuous spectrum; \( \hat{h}(\omega) \) will be a smooth function. The rate of interaction vanishes, but as we take the limit \( t \to \infty \), there is an effective non-zero interaction that is proportional to \( \lambda^2 t \). Recall that

\[ \delta(x) = \lim_{t \to \infty} \frac{1 - \cos(tx)}{t\pi x^2}, \]  

(2.81)

where \( \delta(x) \) is the Dirac delta function, which is defined as \( \int_{-\infty}^{\infty} dx \delta(x) = 1 \) and, \( \forall x \neq 0, \delta(x) = 0 \). With the use of the \( \delta \) function we find

\[ P_{nm,\lambda^2 t} = \delta_{nm}(1 - \lambda^2 t 2\pi \sum_l |S_{ln}|^2 \hat{h}(E_n - E_l)) + \lambda^2 t 2\pi |S_{nm}|^2 \hat{h}(E_n - E_m), \]  

(2.82)

and

\[ \mu_{nm,\lambda^2 t} = e^{it(E_n - E_m)} \left( 1 + \lambda^2 t 2\pi S_{nm}S_{nm} \hat{h}(0) - \lambda^2 t 2\pi g(E_n) - \lambda^2 t 2\pi g^*(E_m) \right), \]  

(2.83)

with

\[ \text{Re} \; g(E_n) = \sum_l |S_{ln}|^2 \hat{h}(E_n - E_l), \]  

(2.84)

and
Im \( g(E_n) = \mathcal{P} \int_{-\infty}^{\infty} d\omega \hat{h}(\omega) \sum_{\ell} \frac{|S_{\ell n}|^2}{\omega - E_n + E_{\ell}} \) \hspace{1cm} (2.85)

where \( \mathcal{P} \) is the principal value of the integral. In order to see in what regime the perturbation theory is correct, we check whether the process described by Eq. (2.82) and Eq. (2.83) corresponds to that of a TCP map. First we verify Property 1 in Eq. (2.83): the eigenvalues of \(|n\rangle\langle m| \) and \(|m\rangle\langle n|\) are related by complex conjugation, or \( P_{mn,\lambda^2 t} = P_{nm,\lambda^2 t} \). The trace-preserving property (also in 1) is also obeyed:

\[ \sum_m P_{mn,\lambda^2 t} = 1. \] \hspace{1cm} (2.86)

Complete positivity of the map implies that \( P_{mn,\lambda^2 t} \) must be a matrix of probabilities, that is we must have \( P_{mn,\lambda^2 t} \geq 0 \). Thus the first necessary condition for the validity of the perturbative approximation is

**Condition 1:** \( \forall \ n : \lambda^2 t \ll \frac{1}{2\pi} \sum_{\ell} \frac{1}{|S_{\ell n}|^2 h(E_n - E_{\ell})} \).

Eq. (2.80) and Eq. (2.87) together ensure that \( P_{mn,\lambda^2 t} \) is a stochastic matrix. Complete positivity also implies via Proposition 4 that \(|\mu_{mn,\lambda^2 t}| \leq 1 \). In order that \( 1 + \lambda^2 t a \leq 1 \), where \( a \) is some complex number, we must have that \( \text{Re } a \leq 0 \) and \( \lambda^2 t \leq 2/|\text{Re } a| \). This real part in Eq.(2.83) is indeed negative as \( \tilde{h}(\omega) \) is positive, and we obtain a new condition:

**Condition 2:** \( \forall \ m, n : \lambda^2 t \ll \frac{1}{|S_{mn} S_{mn} h(0) + \frac{1}{2} \sum_{\ell} |S_{\ell n}|^2 h(E_n - E_{\ell}) + \frac{1}{2} \sum_{\ell} |S_{lm}|^2 h(E_m - E_{\ell})|} \).

Note that this condition is quite similar to the condition in Eq. (2.87).

It is not hard to see that the stochastic matrix \( P_{mn,\lambda^2 t} \) obeys detailed balance for the equilibrium distribution:

\[ P_{mn,\lambda^2 t} e^{-\beta E_n} = P_{nm,\lambda^2 t} e^{-\beta E_m}, \] \hspace{1cm} (2.89)

as the equilibrium condition of the bath implies that

\[ \tilde{h}(\omega) = e^{-\beta a} \tilde{h}(\omega). \] \hspace{1cm} (2.90)

Thus the equilibrium density matrix \( \rho_{a,b} \) is a fixed point of the idealized equilibration process. To consider whether this fixed point is unique, we note the following: If a stochastic matrix \( M \) is such that all its matrix elements \( M_{ij} > 0 \), then \( M \) has a unique eigenvalue equal to 1 \( [\mathbb{6}] \). If Condition 1 is obeyed, we indeed have \( P_{mn,\lambda^2 t} > 0 \) and therefore the absolute value of the second largest eigenvalue (in the diagonal sector) is smaller than 1. For the off-diagonal sector, Condition 2 says that the largest eigenvalue in the off-diagonal sector is strictly smaller than 1 in absolute value. Thus under these conditions, with Proposition 3 we can conclude that the process converges to the equilibrium state. The expression of \( P_{mn,\lambda^2 t} \) coincides with the derivation given by Davies \( [\mathbb{25}] \) for small \( \lambda^2 t \).

One can help to speed up the process in the off-diagonal sector by “dephasing”; that is, after having the system and the bath interact for some time \( t \), we perform the operation

\[ \mathcal{D}^a(\rho_s) = \frac{1}{a} \sum_{s=0}^{a} e^{iH_s s} \rho_s e^{-iH_s s}, \] \hspace{1cm} (2.91)

which can be implemented with the assistance of an extra register in the state \( \frac{1}{\sqrt{a}} \sum_{s=0}^{a} |s\rangle \) which is used to condition the evolution \( U = e^{iH_s s} \) and subsequently traced out. The dephasing has the effect of canceling off-diagonal terms in the eigenbasis of the system, i.e.

\[ \lim_{a \to \infty} \mathcal{D}^a \left( \sum_{k,l} \alpha_{kl} \rho_{kl} \right) = \sum_k \alpha_{kk} \rho_{kk}. \] \hspace{1cm} (2.92)

A complete dephasing can in general not be achieved in polynomial time in \( n \) (see section \( [\mathbb{11}] \)), and thus must be understood as an extra aid but not a solution to the equilibration problem.

From the expressions for \( P_{mn,\lambda^2 t} \) and \( \mu_{mn,\lambda^2 t} \) we can understand the physical picture of the interaction between bath and system. The system makes a transition from (eigen) level \( n \) to level \( m \), when (1) \( S_{mn} \) is non-zero, (2) the bath is capable of “receiving” this quantum of energy \( \Delta E = |E_m - E_n| \), that is, it has a matching energy difference
\[ |\omega_i - \omega_j| = \Delta E \text{ and (3) } B_{ij} \text{ is non-zero. Furthermore, the more such transitions there are, the faster the off-diagonal matrix elements decay. This confirms the intuitive picture that one might have of equilibration. Note also the similarity with the Fermi Golden Rule [22,30] that describes the transition probability from eigenlevel } n \text{ to } m \text{ in a unitary evolution that is perturbed by a time-dependent Hamiltonian.} \]

For a finite-dimensional bath, we can express \( h(t) \equiv (BB_t) \) as

\[
h(t) = \sum_{k,l} e^{it(\omega_k - \omega_l)}|B_{kl}|^2 e^{-\beta \omega_k} / Z_b, \tag{2.93}
\]

where \( B_{kl} = \langle k_b|B|l_b \rangle \) with \( |l_b \rangle \) being the eigenstates of the bath Hamiltonian \( H_b \) and \( Z_b \) the partition function of the bath. Taking the limits \( t \to \infty \) and \( \lambda \to 0 \) before letting the bath grow large leads to divergent expressions for \( P_{nm,\lambda^2t} \) and \( \mu_{nm,\lambda^2t} \), suggesting that the perturbation theory fails in this regime. This is not surprising, as the finiteness of the bath together with the limit \( t \to \infty \) will lead to Poincaré recurrences (only the interaction cycle time is long due to \( \lambda \to 0 \)).

**F. The inverse quantum Zeno effect**

In our numerical studies (sections [1G] and [1H]) we have observed a phenomenon that one might call the inverse quantum Zeno effect. It is a way of mapping an arbitrary initial state onto the completely mixed state \( 1_N \) by interacting repeatedly and strongly with the state for a very short time. Here we will give a theoretical analysis that explains this observation. Consider the weak coupling expansion \( S_{\lambda,t} = S^{(0)}_\lambda + \lambda^2 S^{(2)}_\lambda + \mathcal{O}(\lambda^3) \) with \( S^{(2)}_\lambda \) given as in Eq. (2.71). We expand these operators around \( t = 0 \):

\[
S_{\lambda,t}(\rho) = \rho - i t[H_s, \rho] + \frac{t^2 \lambda^2}{2} (\{S\rho, S\} + [S, \rho S]) \langle B^2 \rangle_b + \mathcal{O}(t^3, \lambda^3 t^3). \tag{2.94}
\]

In the limit \( \lambda \to \infty, \) but \( t \to 0, \) and constant \( \lambda^2 t, \) the higher order terms \( \mathcal{O}(t^2, \lambda^3 t^3) \) will vanish. Thus we see that the fixed point of \( S_{\lambda,t} \) in this limit (assuming non-zero \( \langle B^2 \rangle_b \)) must obey

\[
[H_s, \rho] = 0 \text{ & } \langle [S, \rho], S \rangle = 0. \tag{2.95}
\]

Notice that if we take the differential form of Eq. (2.94) and the prescribed limit, the equation is of the Lindblad form, Eq. (2.17). The state \( 1_N \) certainly meets the requirements of Eq. (2.93), but is it unique? If \( S \) and \( H_s \) are such that they have no eigenspaces (except for the full space) in common, and both have a non-degenerate spectrum, we can show that \( 1_N \) is the unique eigenvector. Eq. (2.93) requires that either \( [S, \rho] = 0 \) or \( [S, \rho] \) is diagonal in the same basis as \( S \). If \( [S, \rho] = 0 \) but also \( [H_s, \rho] = 0 \), then \( \rho \) can only be the state \( 1_N \). What happens if \( [S, \rho] \) is just diagonal in the same basis as \( S \)? Let \( |n \rangle \) be an eigenvector of \( S \) with eigenvalue \( \lambda_n \). We have for \( n \neq m \)

\[
\langle n | [S, \rho] | m \rangle = 0. \tag{2.96}
\]

Rewriting this expression gives

\[
\forall n, m, \; n \neq m \; \langle n | \rho | m \rangle (\lambda_n - \lambda_m) = 0. \tag{2.97}
\]

Now, because \( \rho \) is diagonal in the basis of \( H_s \) as \( [H_s, \rho] = 0 \) and \( H_s \) and \( S \) have no eigenvectors in common, there exist \( n \) and \( m \) such that \( \langle n | \rho | m \rangle \neq 0 \). But the eigenvalues of \( S \) were non-degenerate, thus we obtain a contradiction. \( \square \)

When \( 1_N \) is the unique eigenvector of this process, then, with the use of Proposition 4, the repeated application as in step 4 of the Equilibration algorithm I will eventually bring the system to the state \( 1_N \).

We showed that for this “inverse quantum Zeno” effect to occur \( S \) and \( H_s \) have to be such that they have no partial eigenspace in common and both have a non-degenerate spectrum. If we assume that \( S \) and \( H_s \) are \( c \)-local with \( c \) larger or equal to 4, then this does not impose a very strong constraint on \( S \) and \( H_s \); the effect will occur for a generic \( S \) and \( H_s \).
The main purpose of this study is to understand the effects of bath size and the choice of bath and interaction Hamiltonians for a specific system Hamiltonian. In Table I we list some of the choices that have been made in the numerical analysis. We have randomly generated the elementary Hamiltonians $h_i$ that make up $H_s$, $H_b$ and $H_{sb}$, Eqs. (2.3), (2.5), (2.7), with a measure $M$. We choose the diagonal elements of each $h_i$ uniformly in $[-a,a]$, where $a$ is sampling scale in Table I. The absolute value of the above-diagonal elements of $h_i$ are chosen uniformly in $[0,a]$ and its phase is chosen uniformly in $[0,2\pi]$. The below-the-diagonal elements of $h_i$ follow from Hermiticity. This defines $M$. Note that $M$ is not a unitarily invariant measure.

We take the Hamiltonians $S$ and $B$ as sums of all possible local 2-qubit interactions ($c_s = 4$ in Table I). For the Hamiltonian of the system $H_s$ we also take a sum of all possible local 2-qubit interactions. Note that this includes a set of Hamiltonians that exhibit frustration, for which we don’t expect equilibration to be particularly fast.

In section II E we observed that matching energy differences between bath and system are an important ingredient in the equilibration of the system, which is consistent with the intuitive picture of equilibration that was sketched in section II A. However, as we do not know the eigenvalues of the system, we can only pick our bath so as to optimize the chance for matching level differences. The sampling scale of the bath distribution will be Gaussian (central limit theorem), whereas the system distribution will be similar to a Gaussian distribution for large $N$. Comparing Eqs. (2.101) and (2.103) gives the expression for $a_b$:

$$
|\text{Tr} H_s|_M = |\text{Tr} H_b|_M = 0.
$$

To optimize for matching we choose the variances to be equal:

$$
\frac{|\text{Tr} H_s^2|_M}{N} = \frac{|\text{Tr} H_b^2|_M}{K}.
$$

(2.99)

For large $K$ the bath distribution will be Gaussian (central limit theorem), whereas the system distribution will be similar to a Gaussian distribution for large $N$ (see Fig. 1). Thus, setting the variances equal brings the distributions close together.

Consider first $|\text{Tr} H_s^2|_M$. It is straightforward to calculate the variance of the eigenvalues of a qubit bath. Given a $2 \times 2$ Hermitian matrix $m_{ij}$, the eigenvalues $e_{\pm} = \frac{1}{2}(m_{11} + m_{22} \pm \sqrt{(m_{11} - m_{22})^2 + 4|m_{12}|^2})$ have

$$
[e_{\pm}]_M = \frac{1}{4a^2} \int_{-a}^{a} dm_{11} \int_{-a}^{a} dm_{22} \int_{0}^{2\pi} d|m_{12}| e_{\pm} = \frac{2a^2}{3}.
$$

(2.100)

Let $v_i$ be some $\pm$ pattern of length $k$, corresponding to selecting $e_+$ or $e_-$ for each qubit bath. Let $E_{v_i}$ be an eigenvalue of the full bath, i.e., $E_{v_i} = \sum_{m=1}^{k} e_{v_i[m]}$ where $v_i[m]$ indicates that we select the $m$th bit in $v_i$. Then

$$
|\text{Tr} H_s^2|_M = \frac{1}{K} \sum_{i=1}^{K} |E_{v_i}|_M = \frac{2ka^2}{3}.
$$

(2.101)

We calculate $|\text{Tr} H_s^2|_M = \sum_{i,j} |(H_s)_{ij}|^2 |_M$ for $n > 2$. We can write

$$
\sum_{i,j} |(H_s)_{ij}|^2 = \sum_{i,j} \sum_{m=1}^{\binom{n}{2}} |(h_m)_{ij}|^2 |_M.
$$

(2.102)

where $h_m$ is the $m$th local interaction Hamiltonian. We have used $|(h^*_m)_{ij}(h_m)_{ij}|_M = 0$. Each row of $h_m$ has only four non-zero entries as the dimension of the local Hamiltonians $c_s$ was set to four. Using the fact that $|(h_m)_{ij}|^2 |_M = \frac{1}{3}$ for all interaction terms $m$, we obtain

$$
|\text{Tr} H_s^2|_N = \frac{4}{3} \binom{n}{2}.
$$

(2.103)

For $n = 1$, we have $|\text{Tr} H_s^2|_N = \frac{2}{3}$. Comparing Eqs. (2.101) and (2.103) gives the expression for $a_b$.
\[ a_b = f(n, k, 4, 2) = \sqrt{\frac{2}{k} \binom{n}{2}}. \]  

For \( n = 1 \), \( f(1, k, 4, 2) = \sqrt{1/k} \). Fig. [ ] illustrates how this setting determines the density of states of bath and system.

The numerical work consists of a calculation of the fixed point of \( S_{\lambda,t} \) as a function of \( t \) for a fixed \( \lambda \) and the second largest eigenvalue for different baths and different systems and temperatures. We follow a numerical procedure based on perturbation theory (Section II D) to perform a stable numerical evaluation of these quantities. We can trust the answers from the numerical procedure only if we are in the regime in which perturbation theory is correct. This regime was heralded by the two conditions Eq. (2.87) and Eq. (2.88) in section II. Whether these conditions are obeyed depends on the specific choices of \( H_s, H_b \) and \( S \) and \( B \). We prefer to reformulate these conditions here such that they are obeyed for the average bath, system and interaction Hamiltonian obtained by sampling using \( M \) and the sampling scale. As the conditions are very similar, we take the first one, Eq. (2.87), and reformulate it as

\[ c(t) \equiv \lambda^2 t 2\pi \frac{NK[S^2]_M[B^2]_M}{W_b} \leq 1. \]  

where \([S^2]_M\), the average matrix element, is defined as

\[ [S^2]_M = \frac{1}{N^2} \sum_{i,j} |S_{ij}|^2 = \frac{1}{N^2} [\text{Tr}_s S^2]_M, \]  

and similarly for \([B^2]_M\). \( W_b \) is the spectral width of the bath, i.e.,

\[ W_b^2 = \frac{[\text{Tr}_b H^2]_M}{K}. \]  

Here we indicate the approximations made in obtaining Eq. (2.105) from Condition 1 (Eq. (2.87)):

\[ \lambda^2 t 2\pi \sum_l |S_{ln}|^2 \hat{h}(E_n - E_l) \ll 1. \]  

Using Eq. (2.93) and Eq. (2.73) we write the \( \hat{h} \) function as

\[ \hat{h}(E_n - E_l) = \sum_{k,m} \delta((E_n - E_l) - (\omega_k - \omega_m)) |B_{km}|^2 e^{-\beta \omega_k}/Z. \]  

We will approximate the matrix elements \(|B_{kl}|^2\) as constants and replace them by their average \([B^2]_M\). Then we can use density-of-states arguments to approximate the \( m \) sum over the \( \delta \) functions by the inverse of the average spacing between the \( \delta \) functions; this spacing is given by \( W_b/K \):

\[ \sum_m \delta((E_n - E_l) - (\omega_k - \omega_m)) \approx \frac{K}{W_b}. \]  

With these approximations, the partition-function sum over \( k \) in Eq. (2.103) becomes exactly one. So, Eq. (2.109) becomes

\[ \hat{h}(E_n - E_l) \approx \frac{K[B^2]_M}{W_b}. \]  

Now Eq. (2.108) is

\[ \lambda^2 t 2\pi \frac{K[B^2]_M}{W_b} \sum_l |S_{ln}|^2 \ll 1. \]  

If we again approximate the matrix elements \(|S_{ln}|^2\) as constants and replace them by their average \([S^2]_M\), and note that the \( l \) sum in Eq. (2.112) has \( N \) terms, we obtain Eq. (2.103).

For the simulations we have performed, we can find the values for \([S^2]_M\) and \([B^2]_M\) (note that these Hamiltonians have locality parameter \( c = 4 \), as does the system Hamiltonian \( H_s \)) and obtain the expression
\[ c(t) = \lambda^2 t \frac{16\pi}{3\sqrt{3}} \left( \frac{k}{2} \right) \sqrt{\left( \frac{n}{2} \right)} \ll 1. \] (2.113)

for \( n > 1 \) and \( k > 1 \). For a qubit system, \( n = 1 \), and \( k > 1 \) we obtain

\[ c_1(t) = \lambda^2 t \frac{8\pi\sqrt{2}}{3\sqrt{3}} \left( \frac{k}{2} \right) \ll 1. \] (2.114)

The quantity \( c(t) \) in Eq. (2.105) will function as a rescaled time which depends on the strength of \( \lambda \) and the size of system and bath. In the regime where \( c(t) \leq 1 \) we expect a perturbative calculation of the eigenvectors and eigenvalues of the superoperator to be fairly accurate. The dimensionless parameter associated with the temperature is given by

\[ \beta' = \beta W_s, \] (2.115)

where \( W_s \) is the spectral width of the system, Eq. (2.107) \((W_s = W_b)\). From here on, \( \beta \) will refer to this scaled dimensionless parameter. Instead of expanding the superoperator \( S \) in a series in \( \lambda \) as in Eq. (2.47), we write

\[ \lambda^2 S^{(2)}_t = S_{\lambda,t} - S^{(0)}_t, \] (2.116)

where all higher order terms are grouped in \( \tilde{S}^{(2)}_t \). The calculation of eigenvalues and eigenvectors then follows the analysis of Section II D. We find that the choice for the bath and the interaction Hamiltonian influences whether the equilibration will succeed or not. Let

\[ D = \| \rho_{s,\beta} - \rho_0 \|_{tr}, \] (2.117)

where \( \rho_0 \) is the unit eigenvector obtained from the numerics. In Figs. 2 and 3 two extrema in dynamics are shown, each corresponding to a different choice for the system, bath, and interaction. In Fig. 2 the equilibration is successful, whereas in Fig. 3 the equilibration fails. \( R_D \) is defined as

\[ R_D = \frac{1 - |\kappa_D|}{\bar{c}(t)}, \] (2.118)

where \( \kappa_D \) is the second largest eigenvalue in the diagonal sector and \( \bar{c}(t) \) is the average coupling strength in the time interval that we consider, which is \( c(t) \in [0, 0.3] \) here. Similarly, we define

\[ R_{ND} = \frac{1 - |\kappa_{ND}|}{\bar{c}(t)} \] (2.119)

for the nondiagonal sector.

### H. Numerical results for equilibration

We are interested in how well a randomly chosen bath and interaction equilibrate a system and how these averages are improved by choosing larger baths. As the mixing rates and the distance to the equilibrium state will in general be oscillating functions of the scaled time \( c(t) \) (see Fig. 3) we will compute time averaged rates over a reasonable interval in \( c(t) \),

\[ [c(t_{init}) = 0, c(t_{end}) = 0.5], \] (2.120)

such that we are in the realm where perturbation theory is valid, Eq. (2.102). We denoted these time averages (not to be confused with bath averages) as \( \overline{R_D} \) and \( \overline{D} \) for the time averaged trace distance, Eq. (2.117), etc. In Fig. 4 we present histograms that show how, for a given fixed system and interaction, the equilibration process is different for a set of randomly chosen baths with fixed dimension. The insets show the distribution for the lowest bin. The vertical axis denotes the percentage of baths (the interval \([0\%, 100\%]\) is given as the interval \([0, 1]\)) for a certain distance and rate. We observe that the diagonal rate distribution is very broad, and therefore the mean of the distribution is not a very good (or a very stable) measure of the generic behavior. Furthermore, we find that the rate in the diagonal sector is much worse than in the nondiagonal sector and thus is the dominant factor in setting the mixing time. This
conforms to the pattern in many quantum systems, for example for nuclear spins as observed by NMR, for which \( T_1 \) is generically larger than \( T_2 \) [33].

To study the dependence on \( \beta \) and on the dimension of the bath versus the dimension of the system, we compute the following data. We pick a system Hamiltonian \( H_s \) of \( n \) qubits that has some well spread out spectrum. We set the dimension of the bath and then we randomly pick both the bath Hamiltonian and the interaction Hamiltonian. Means are denoted as \([\mu]_{M_b}\). For the rates we look both at the mean and the median. The median is denoted as \([\mu]_{M_b}\), see Fig. 3. The results for \( n = 1, 2, 3 \) and 4 are shown in Figs. 3-8. We have given the median when the mean does not give a good representation of the distribution.

These data clearly indicate that larger baths improve the process of equilibration, both in the rates (D and ND) as well as in the closeness to the equilibrium state. The effects are the most pronounced at low temperature, where equilibration is in general harder as the system must relax to a single pure ground state. To understand the closeness scale, we show in Appendix A how far apart two arbitrarily chosen density matrices are; this number lies around 1 for the dimensions that were considered. For these estimates, we see a trend towards approximations getting worse for larger system sizes for low temperature. The scaled rates \([\mathcal{R}_{D}, M_b]_{M_s}\) and \([\mathcal{R}_{ND}, M_b]_{M_s}\) seem to be fairly constant, thus we see behavior that suggests that the rates are polynomially related to both system and bath number of qubits. We also observe that the nondiagonal rate (ND) is always higher than the diagonal rate (D). The data show a system Hamiltonian dependence, that is, the average equilibration for \( n \) is \( \beta \) and on the dimension of the bath versus the dimension of the system, we compute

\[
\mathcal{R}_{T_{\beta}, n}\]

(3.3)

where \( p_{st}^\beta = e^{-\beta(t-s)} \).

III. EQUILIBRATION II

We present an alternative to the algorithm in section II. This algorithm relies on the technique for the estimation of eigenvalues, originally given in [2] (see [37,38]). This eigenvalue estimation routine has also been used as a building block in an interesting quantum algorithm in [39] and [40].

Let \( H_s \) be the \( c \)-local Hamiltonian with non-degenerate eigenvalues as in section II. Order the eigenvalues as \( E_0 > E_1 > \ldots > E_N \).

**Definition 2** Equilibration algorithm II.

1. **Initialize** the system in the (infinite temperature) completely mixed state \( 1_N \). Also add one \( m \)-qubit register set to \( |00\ldots00\rangle \).

2. **Compute eigenvalues** with the use of the Fourier transform and dephase in computational eigenvalue basis, which will result in state

\[
\sum_{n=0}^{N-1} \sum_{s=1}^{2^n-1} p(s,n) |n\rangle |s\rangle \otimes |s\rangle |s\rangle,
\]

where \( p(s,n) \) is a distribution, peaked at \( s \sim E_n \) for large \( m \). The dephasing is a simple superoperator \( \mathcal{D} \) on the eigenvalue register that operates as

\[
\mathcal{D}(|s_i\rangle |s_i\rangle) = |s_i\rangle |s_i\rangle, \quad \mathcal{D}(|s_i\rangle |s_j\rangle) = 0.
\]

3. **Prepare** an additional \( N \)-dimensional quantum system, the bath, also in \( 1_N \). Add a \( m \)-qubit register and one qubit register set to \( |00\ldots00\rangle \).

4. **Compute eigenvalues** of the bath as for the system in step 2.

5. **Interact** system and bath according the following rule \( \mathcal{R} \) ("partial swap"):

\[
U_{\mathcal{R}} |n,m\rangle |s,t\rangle = \begin{cases} |m,n\rangle |s,t\rangle |0\rangle & \text{if } t < s \\ (p_{st}^{\beta/2} |t,s\rangle |0\rangle + \sqrt{1 - p_{st}^{\beta}} |s,t\rangle |1\rangle) |s,t\rangle & \text{if } t \geq s \end{cases}
\]

where \( p_{st}^\beta = e^{-\beta(t-s)} \).
6. **Trace** over the single-qubit register, all bath registers, and the eigenvalue register of the system. The system will be in some state

\[ \rho_s = \sum_n \alpha_n |n\rangle \langle n| \].

(3.4)

The steps 2-6 define a TCP map \( S, S(1_N) = \rho_s \).

7. **Repeat** steps 2-6 \( r \) times such that

\[ \| S^{r+1} (|000\ldots00\rangle |000\ldots00\rangle) - S^r (|000\ldots00\rangle |000\ldots00\rangle) \|_{tr} \leq \epsilon, \]

(3.5)

for all \( r \geq r_0 \) and \( \epsilon \) is some accuracy.

The advantage of this algorithm is its simplicity and its similarity to a classical algorithm; we create a Markov chain in the eigenbasis of the system. The disadvantage of the algorithm is that it is very likely to be slow; the computation of the eigenvalues to high accuracy with the use of the Fourier transform is very likely to be exponential in the number of qubits of the system and has to be performed twice, for system and bath, in each round of the chain. First, let us show that in the case when the eigenvalues are computed exactly in steps 2 and 4, i.e, for all \( \alpha_n \) such that

\[ \sum_n \alpha_n (|n\rangle \langle n|) \],

(3.6)

where \( \alpha_m^{(k)} = \sum_n \alpha_n^{(k-1)} p_{n \rightarrow m} \). We have

\[ P_{n \rightarrow m} = \begin{cases} \frac{1}{N} & \text{if } E_m < E_n \\ \frac{1}{N} (1 + \sum_{k \leq n} (1 - p_{nk}^2)) & \text{if } E_m = E_n \\ \frac{1}{N} p_{nm}^2 & \text{if } E_m > E_n \end{cases} \]

(3.8)

Note that \( \sum_m P_{n \rightarrow m} = 1 \) as required. The equilibrium state Eq. (1.1) obeys the detailed balance condition:

\[ \forall n, m \quad P_{n \rightarrow m} e^{-\beta E_n} = P_{m \rightarrow n} e^{-\beta E_m}. \]

(3.9)

All the matrix elements of the Markov matrix \( P_{n \rightarrow m} \) are nonzero. Therefore the chain will have a unique fixed point which is equal to the equilibrium state due to detailed balance. Thus for all probability distributions \( \alpha_n \) we have

\[ \lim_{k \rightarrow \infty} \sum_n \alpha_n P_{n \rightarrow m}^{(k)} = \frac{e^{-\beta E_m}}{Z}. \]

(3.10)

Notice that it is not hard to prepare the initial states of system and bath. One way to make the completely mixed state \( 1_N \) is to make a maximally entangled state \( \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle |i\rangle \) and trace over the second register. This takes \( O(n) \) steps. The partial swap in step 5 can be implemented with \( O(n) \) elementary qubit steps. The dephasing in step 2 is introduced to keep the form of the algorithm clean, but it does not affect its output. This dephasing is implemented by measuring the eigenvalue register in the computational basis and discarding its answer. When using an \( m \)-bit eigenvalue register the joint probability \( p(n, s) \) in the first round (after step 2) is equal to

\[ p(n, s) = \frac{1}{N} \left| \frac{1}{2^m} \sum_{i=0}^{2^m-1} e^{i(E_n - 2\pi s/2^m)} \right|^2. \]

(3.11)

When \( p(n, s) \) is not a delta function on the eigenvalue, the Markov chain will still be in the eigenbasis of the system; it will be a concatenation of chains; the transition probability of this new chain is
where $p(s|n)$ is a conditional probability, defined by $p(n, s) = p(s|n)p(n)$, and $P_{s \rightarrow t}$ is the exact chain (when $p(s|n) = \delta_{E_{s}, s}$). Note that $\sum_{s} p(s|n) = 1$ and $\sum_{n} p(m|t) = 1$, so that $P'_{n \rightarrow m}$ is a stochastic matrix. Let us make a few remarks about the behavior of such an approximate equilibration process. If this new Markov chain is close to the exact Markov chain, we can bound the deviation from the exact fixed point with perturbation theory \[40\]. Let

\begin{equation}
\rho_{n \rightarrow m} = P_{n \rightarrow m} + E_{nm},
\end{equation}

where $E_{nm}$ is a deviation matrix defined by Eq. \[3.12\]. Let $\rho_{\Delta} = \rho'_{s, \beta} - \rho_{s, \beta}$ where $\rho'_{s, \beta}$ is the fixed point of the Markov chain $P'_{nm}$. Assume that $P$ is diagonalizable. Let $Y$ be the matrix defined as

\begin{equation}
Y = (1 - P + P^{(\infty)})^{-1} - P^{(\infty)},
\end{equation}

where $P^{(\infty)}$ is the infinite iteration of $P$. We can write $P^{(\infty)} = \text{diag}(1, 0, \ldots, 0)$ in the basis where the stationary state $\rho_{s, \beta}$ is an eigenvector. In this basis, with diagonalizability, $P$ is of the form $\text{diag}(1, \lambda_{2}, \ldots, \lambda_{N})$. We can then write

\begin{equation}
Y = \text{diag}(0, \frac{1}{1 - \kappa}, \ldots, \frac{1}{1 - \lambda_{N}}),
\end{equation}

where $\kappa$ is the second largest eigenvalue. For later use we note that the norm $\| Y \|_{2} = \frac{1}{|1 - \kappa|}$. It is possible to write the deviation $\rho_{\Delta}$ in terms of $Y$ and $E$:

\begin{equation}
\rho_{\Delta} = (1 - YE)^{-1}YE\rho_{s, \beta}
\end{equation}

when $E$ is small enough such that $1 - YE$ is invertible. This expression can be derived from $P^{(\infty)}\rho_{\Delta} = 0$, which follows from the uniqueness of the stationary state $\rho$. We now use

\begin{equation}
\| \rho_{\Delta} \|_{tr} \leq \sqrt{N} \| \rho_{\Delta} \|_{2},
\end{equation}

as in Proposition \[3\]. Then using the expression for $Y$, Eq. \[3.16\] and Eq. \[3.17\] (see also below Eq. \[2.37\]) we can bound

\begin{equation}
\| \rho_{\Delta} \|_{tr} \leq C_{N} \text{Tr} \rho_{s, \beta}^{2} \left( \frac{1 - \| E \|_{2}}{1 - \kappa} \right)^{-1} \frac{\| E \|_{2}}{1 - \kappa} \leq C_{N} \left( 1 - \frac{\| E \|_{2}}{1 - \kappa} \right)^{-1} \frac{\| E \|_{2}}{1 - \kappa},
\end{equation}

Thus the size of the correction $\rho_{\Delta}$ will be determined by the strength of the perturbation $\| E \|_{2}$ and the rate of convergence of the original Markov chain $P$.

For a general $H_{s}$, the computation of an $m$-bit approximation of the eigenvalues is likely to cost an exponential (in $m$) number of elementary gates. As there are $2^{n}$ eigenvalues, knowing the $m = \log \text{poly}(n)$ bits of the values of $E_{n}$ still leaves groups of $\frac{2^{n}}{\text{poly}(n)}$ eigenvalues indistinguishable. Thus only in very special cases, if the gates $U_{s}^{2^{m}}$ can be implemented with a polynomial (in $m$) number of elementary steps (as in Shor’s factoring algorithm \[1\]) it is possible to compute the eigenvalues to high accuracy efficiently.

We have demonstrated a way to set up a Markov chain on a quantum computer that will converge to the equilibrium state for long enough time. For special Hamiltonians, there might be more efficient ways to tune and modify this kind of algorithm. The rule $R$ might be chosen to depend on other features of the eigenstates $|n\rangle$ and $|m\rangle$ as in the classical Metropolis algorithm where transitions are made between states that are related by local spin flips. There might be Hamiltonians for which the calculation of an eigenvalue, given the eigenvector, is efficient. Then there is the hard question of the (rapidly) mixing properties of the chain, that determines the computational efficiency of the algorithm.

IV. (TIME-DEPENDENT) OBSERVABLES

Given that we have prepared $n$ qubits in the equilibrium state corresponding to a certain Hamiltonian $H_{s}$, we can then proceed by experimenting and measuring. The simplest measurement that we could try to perform is the estimation of the expectation value of a $c$-local (Hermitian) observable $O$: 

\[21\]
\[ \langle O \rangle_s = \text{Tr} \, \rho_{s,\beta} \, O. \] (4.1)

As \( O \) is local, we write \( O = \sum_{i=1}^{\text{poly}(n)} O_i \), where each operator \( O_i \) operates on a Hilbert space of constant dimension \( c \). We can calculate the eigenvectors and eigenvalues of each \( O_i \) rapidly on a (possibly) classical computer, which takes \( \text{poly}(n, c) \) operations. If \( O_i \) has eigenvalues \( \mu_i \) that are both smaller as well as larger than zero, we define \( O_i^+ \) as

\[ O_i^+ = \frac{1}{\max_k \mu_k + |\min_k \mu_k|} (O_i + |\min_k \mu_k| I) \] (4.2)

such that \( O_i^+ \) is positive semi-definite and has eigenvalues smaller than or equal than 1. If \( O_i \) has only positive or zero eigenvalues, we just “normalize” the operator by dividing by \( \max_k \mu_k \), and similarly if \( O \) has only negative eigenvalues. Let \( I \) be a positive operator valued measurement (POVM [41]) with operation elements \( A_{1,i} \) and \( A_{2,i} \) and corresponding outcomes 1 and 2 such that

\[ E_{1,i} = A_{1,i}^+ A_{1,i} = O_i^+, \]
\[ E_{2,i} = A_{2,i}^+ A_{2,i} = 1 - O_i^+. \] (4.3)

This measurement will give outcome 1 with probability
\[ p_{1,i} = \text{Tr} \, O_i^+ \rho \] etc. (4.4)

The operators \( A_{1,i} \) and \( A_{2,i} \) are given by

\[ A_{1,i} = U_\alpha (\text{diag}_{O_i^+})^{1/2} U_\alpha^\dagger \quad \text{and} \quad A_{2,i} = U_\alpha (1 - \text{diag}_{O_i^+})^{1/2} U_\alpha^\dagger, \] (4.5)

where \( \text{diag}_{O_i^+} \) is the diagonal form of \( O_i^+ \) and \( U_\alpha \) the diagonalizing matrix. We summarize these results in a Proposition:

**Proposition 5** The estimation of \( \text{Tr} \, \rho \, O \) where \( O \) is a c-local observable with precision \( \delta \) and error-probability \( \epsilon \) and \( \rho \in B_{\text{pos,1}}(H_N) \) \( (N = 2^n) \) takes \( T \, O(\ln \frac{1}{\epsilon} / \delta^2) \text{poly}(n, c) \) operations where \( T \) is the time to prepare the state \( \rho \).

**Proof:** All commuting observables \( O_i \) can be measured once for a single preparation of \( \rho \). To estimate a probability \( p \) with precision \( \delta \) and error probability \( \epsilon \) we need \( O(\ln \frac{1}{\epsilon} / \delta^2) \) samples [42].

More interesting is an algorithm to estimate time-dependent expectation values. Let \( O_1 \) and \( O_2 \) be two c-local observables. We consider how to estimate a time-dependent quantity (identical to Eq. (1.10))

\[ \text{Tr} \, \rho_{\beta} \, [O_1, O_{2t}], \] (4.6)

where \( O_{2t} \) is in the Heisenberg representation. Notice that \( O_{2t} \), the time-evolved operator, will for general \( t \) not be local. Thus we cannot use Proposition 3. The way these quantities come about in linear response theory [11] provides the key for how to estimate them on a quantum computer. One considers a system that is perturbed at some initial time \( t = 0 \): its time evolution is generated by the perturbed Hamiltonian \( H_0 + \lambda O_1(t) \) \( (O_1(t < 0) = 0) \) and \( \lambda \) is small. After time \( t \) we consider the response of the system to the perturbation by measuring another observable \( O_2 \). Notice that with Proposition 3, it is simple to perform this experiment. Linear response means that we take into account corrections of order \( \lambda \), but no higher order, in the estimation of

\[ \delta \langle O_2 \rangle_s = \text{Tr} \, O_2 \rho_t - \text{Tr} \, O_2 \rho_{\beta}, \] (4.7)

where \( \rho_t \) is the time-evolved system density matrix. This first-order correction takes the form [36]

\[ \delta \langle O_2 \rangle_s \approx i \lambda \int_0^t dt' \, \text{Tr} \, \rho_{\beta} \, [O_1(t'), O_{2t-t'}]. \] (4.8)

If the disturbance \( O_1(t) = O_1 \delta(t = 0) \) we find on the right hand side the correlation function of Eq. (4.0). The quantity of Eq. (4.0) is interesting, because it can be used to compute the simplest response of the system, the linear response of Eq. (4.8), which we can directly estimate on our quantum computer, provided that both \( O_1 \) and \( O_2 \) are local. But we are of course not restricted to a linear response regime: \( \lambda \) is a parameter that we can tune freely. A sequence of measurements could determine higher response functions that will involve quantities such as

\[ \langle O_{1t_1} O_{2t_2} O_{3t_3} \ldots O_{kt_k} \rangle_s. \] (4.9)
V. CONCLUSION

It seems that by asking the question of how fast real quantum systems equilibrate, we have opened a Pandora’s box of hard-to-answer questions. If there are many simple quantum systems in nature that equilibrate slowly (that is, not in polynomial time) by any dynamics that does not require extensive preknowledge of the system, then it would be unreasonable to ask our quantum computer to perform this task efficiently. By relaxation in polynomial time we mean the following: in polynomial time we obtain a state that is within $\epsilon$ trace distance of the equilibrium state where $\epsilon$ is a small constant. It might be the case that leaving aside the classical phenomenon of frustration, relaxation does not take place in polynomial time. The idea here is that for a quantum system, the eigenbasis is not known beforehand, but must be singled out on the basis of an estimation of the eigenvalues, which is generically a hard problem.

This however is not in contradiction with physical and experimental reality as we know it, as the quantities that are measured in an experimental setup usually involve operators on a small number of qubits; these are the experiments that can be done efficiently (in polynomial time) and thus do not necessarily probe the system’s complete state. For example, the outcomes of the set of measurements $\sigma_{i_1} \otimes \sigma_{i_2} \otimes \ldots \sigma_{i_n}$, where $\sigma_{i_j}$ is one of the Pauli matrices or 1, completely determines the state, but there are $4^n$ measurements in this set. In an experimental setup, we might randomly select a polynomial subset of them and there is some small chance of order $\frac{\text{poly}(n)}{4^n}$ that these are the measurements that distinguish the equilibrated state from the present state in the lab that is supposed to approximate it. The estimates of time-dependent correlations could possibly be more sensitive to distance from equilibrium, as these involve time-evolved, non-local operations. The numerical study suggests that product baths whose size is polynomially related to the system can function as adequate baths in the sense of providing relaxation in polynomial time. The relaxed state could still be a rather rough approximation to the true equilibrium state, but, as we argued above, it might be a good starting point for subsequent measurements.

We have taken the bath to be part of the (cost of) the quantum computer. In any experimental setup, there is a natural bath that is used to equilibrate and cool the quantum computer. Can we use this bath for a computational problem such as equilibration? Consider for example the NMR quantum computer [18] where computation takes place at room temperature. In the regime in which the heat bath has a non-Markovian character it has been shown to be possible to alter the Hamiltonian of the system and the coupling to the bath dynamically (see [43], but also standard books on NMR [33]). These techniques could make it possible to simulate the time-evolution of a “designer” Hamiltonian and also to equilibrate the system to the equilibrium state of this designer Hamiltonian.

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APPENDIX A: NORMS

In this Appendix we give the definitions of several norms and inner products. The inner product between vectors in $\mathbb{C}^{N^2}$ can be represented on $B(\mathcal{H}_N)$ as

$$\langle \chi_1 | \chi_2 \rangle = \text{Tr} \chi_1^\dagger \chi_2.$$

The trace norm [34,35] is defined as

$$\| A \|_{tr} = \text{Tr} \sqrt{A^\dagger A}.$$  \hfill (A2)

What makes this norm attractive is that it captures a measurable closeness of two density matrices $\rho_1$ and $\rho_2$ [33]:

$$\| \rho_1 - \rho_2 \|_{tr} = \max_A \sum_j |P_1^A(j) - P_2^A(j)|,$$

where $P_1^A$ and $P_2^A$ are the probability distributions over outcomes $j$ that are obtained by measuring observable $A$ on $\rho_1$ and $\rho_2$. The matrix norm $\| . \|_2$ is defined as

$$\| A \|_2 = \max_{x, \| x \|_2 = 1} \| Ax \|_2.$$

\hfill (A4)
where \( \| \cdot \|_2 \) is the Euclidean norm on \( \mathbb{C}^{N^2} \): \( \sqrt{\langle v|v \rangle} \) for \( |v \rangle \in \mathbb{C}^{N^2} \). We have
\[
\|Ax\|_2 \leq \|A\|_2 \cdot \|x\|_2.
\]

In order to aid in the interpretation of the numerical results of section 11, we present some numerical estimates for the average \( \| \cdot \|_{tr} \) distance of two randomly chosen density matrices. We first have to choose a measure over \( B_{pos,1} \). All density matrices can be written as \( \rho = \sum_i \lambda_i \rho_{ii} \) with \( \sum_i^N \lambda_i = 1 \). The eigenvalues \( \lambda_k \) lie on a \( (N-1) \)-dimensional simplex \( S \) in \( \mathbb{R}^N \). We use the Euclidean metric \( \| \cdot \|_2 \) induced on the simplex. The Haar measure on the group of unitary matrices \( U(N) \) induces a uniform measure on the set of projectors \( \{ \rho_{ii} \}_{i=1}^{N^2} \). Together this defines a measure \( M_{B_{pos,1}} \). Within this measure, one can express the average distance between two density matrices \( \rho_1 \) and \( \rho_2 \), using the unitary invariance of \( \| \cdot \|_{tr} \), as
\[
\| \rho_1 - \rho_2 \|_{tr, B_{pos,1}} = \frac{1}{\text{Vol}(S)^2 V(U(N))} \int dU \int_0^1 d\lambda_1 \cdots d\lambda_k \int_0^1 d\mu_1 \cdots d\mu_k \delta(\sum_i \lambda_i - 1) \delta(\sum_i \mu_i - 1) \frac{\text{Tr}[\sum_j \lambda_j \rho_{jj} - U \sum_j \mu_j \rho_{jj} U^\dagger]}{Z_i}.
\]

The values obtained by a numerical calculation of Eq. (A4) are tabulated in Table 1.

**APPENDIX B: PREPARATION OF THE BATH**

To prepare the state
\[
\rho_{b,\beta} = \rho_{b,\beta}^1 \otimes \cdots \otimes \rho_{b,\beta}^k,
\]
given \( H_b = \sum_{i=1}^k 1_{K/2} \otimes h_i \), we first calculate the eigenvalues and eigenvectors of each qubit Hamiltonian \( h_i \). We prepare the state
\[
\Pi_{i=1}^k \left( e^{-\beta\epsilon_{i,0}|0\rangle\langle 0|} + e^{-\beta\epsilon_{i,1}|1\rangle\langle 1|} \right) / Z_i.
\]
with \( \{\epsilon_{0,i}, \epsilon_{1,i}\} \) the eigenvalues of qubit Hamiltonian \( h_i \). This can be done by changing an initial state \(|0\rangle\langle 0|\) with probability \( e^{-\beta\epsilon_{i,1}}/Z_i \) into state \(|1\rangle\langle 1|\) for each \( i \). We then rotate each qubit to its eigenbasis \( \{|b_{i0}\rangle, |b_{i1}\rangle\} \):
\[
\otimes_{i=1}^k U_{b_i} = \otimes_{i=1}^k (|b_{i0}\rangle\langle 0| + |b_{i1}\rangle\langle 1|).
\]

In total we perform \( 2k \) elementary qubit operations plus some constant classical overhead.

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|                | \(H_a\) | \(H_b\) | \(S\) | \(B\) |
|----------------|---------|---------|-------|-------|
| dimension      | \(N = 2, \ldots, 2^k\) | \(K = 2^k, \ldots, 2^n\) | \(N\) | \(K\) |
| locality       | \(c_s = 4\) | \(c_b = 2\) | \(4\) | \(4\) |
| sampling scale | \(1\)   | \(f(n, k, c_s, c_b)\) | \(1\) | \(1\) |

**TABLE I.** Some settings in the numerical simulation.
FIG. 1. A histogram (500 samples) of the density of states (unnormalized) for $N = 32$ and $K = 64$ with sampling scale set as Eq. (2.104).
FIG. 2. An example of successful equilibration for $n = 1$, $k = 3$ and $\beta = 3$. 
FIG. 3. An example of an unsuccessful equilibration for $n = 1$, $k = 3$ and $\beta = 3$. 
FIG. 4. An example of the distribution of baths (500 samples) for $n = 2$ and $k = 3$ and $\beta = 2$. 
FIG. 5. Means and median for $n=1$ (500 samples).
FIG. 6. Means for $n=2$ (200-500 samples).
FIG. 7. Means for n=3 (50-100 samples).
FIG. 8. Means for n=4 (15-20 samples).
| dim N | mean    | standard error $= \sqrt{\text{var}/(n - 1)}$, $n = 1000$ |
|-------|---------|------------------------------------------------------|
| 4     | 0.90388 | 0.00740588                                           |
| 8     | 0.96190 | 0.00514057                                           |
| 16    | 1.00294 | 0.00341226                                           |
| 32    | 1.01452 | 0.00220363                                           |
| 64    | 1.02617 | 0.00132233                                           |

TABLE II. The average distance between two randomly selected density matrices.