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Thermalizing Quantum Machines: Dissipation and Entanglement

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We study the relaxation of a quantum system towards the thermal equilibrium using tools developed within the context of quantum information theory. We consider a model in which the system is a qubit, and reaches equilibrium after several successive two-qubit interactions (thermalizing machines) with qubits of a reservoir. We characterize completely the family of thermalizing machines. The model shows a tight link between dissipation, fluctuations, and the maximal entanglement that can be generated by the machines. The interplay of quantum and classical information processes that give rise to practical irreversibility is discussed.

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The hypothesis of the quantum appeared suddenly in physics as an offspring of thermodynamics, due to the work of Planck on the blackbody radiation. In its early days, however, the new theory developed rather as a form of reversible mechanics. One century after Planck's intuition, the link between quantum mechanics (QM) and thermodynamics has been discussed by several scientists, and is still an actual field of research [1]. In parallel to fundamental issues, the concept of *quantum machines* has arisen recently in the field of quantum information processing [2]. Looking back again to history, we see that thermodynamics was born to describe engines. It is thus natural to ask whether there is a "thermodynamics" of quantum machines, and whether the modern standpoint of quantum information can cast some new light on the foundations of thermodynamics. After some pioneering works [3], these ideas have stimulated many investigations in the last months [4].

In this Letter, we focus on the process of *thermalization*, that is, the relaxation towards the thermal equilibrium of a system in contact with a huge reservoir (bath). More precisely, let ρ_B be the thermal state of the bath [5], ρ a generic state of the system, and ρ^e the state of the system at thermal equilibrium. A thermalization process is defined by these two requirements: (I) The state $\rho^e \otimes \rho_B$ is stationary; (II) if the system is prepared in a state $\rho \neq \rho^e$, at the end of the process we have a total state ρ_{SB} such that $\text{Tr}_B[\rho_{SB}] \simeq \rho^e$ and $\text{Tr}_S[\rho_{SB}] \simeq \rho_B$, where $\text{Tr}_{B,S}$ are the partial trace over the bath and the system, respectively.

Thermalizing quantum channels can be realized by letting the system undergo interactions with the bath that are localized in time. Such models, known as *collision models* [6], are admittedly rather artificial as models for dissipative processes [7], but are most natural in the context of quantum information [8]. The system passes through several identical machines U (Fig. 1), or several times through the same machine; at each passage, it becomes entangled (that is, it shares a part of the information encoded in the state) with an ancilla, i.e., some degrees of freedom of the

bath. At the output of the machine, the ancilla is discarded into the bath: the information present in the system has undergone some degradation that depends on the state of the bath and on the machine.

Our main goal is to quantify the role of *entanglement* in this thermalization process. Since a computable measure for entanglement of mixed states is known only for states of two two-dimensional quantum systems (qubits) [9], we consider a thermalization process in which both the system and the ancillas are qubits. Before discussing entanglement, we give the family of all the *thermalizing machines* U acting on two qubits, and a fluctuation-dissipation theorem for the thermalizing channel that these U define.

The model.—We start with a description of the model:

(i) The system is a qubit, and the bath is a reservoir composed of an arbitrarily large number N of qubits. The free Hamiltonian for the whole system is

$$H_0 = H_S + H_B = h[S] + \sum_{i=1}^N h[i], \quad (1)$$

where $h[k]$ is the operator acting as $h = -E\sigma_z$ on the qubit k and trivially on the other qubits. The bath is supposed to be initially in the thermal state $\rho_B = e^{-\beta H_B} / \text{Tr}(e^{-\beta H_B}) = (\xi)^{\otimes N}$ with $\xi = e^{-\beta h} / \text{Tr}(e^{-\beta h}) = \frac{1}{2}[\mathbb{1} + \tanh(\beta E)\sigma_z]$, and $\beta = \frac{1}{kT}$. Let $P_0 = |0\rangle\langle 0|$ and $P_1 = |1\rangle\langle 1|$ be the projectors on the eigenstates of σ_z ; thus

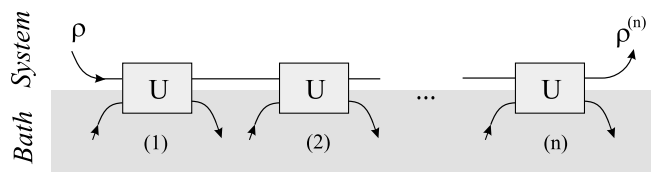


FIG. 1. The quantum channel: a repeated application of a unitary U (quantum machine), that couples the state of the system with the state of the bath.

$$\xi = pP_0 + qP_1, \quad q = 1 - p, \quad (2)$$

with $p = \frac{1}{2}[1 + \tanh(\beta E)]$. We set $E > 0$, so that $|0\rangle$ is the ground state, and $p = 1$ corresponds to $T = 0$.

(ii) The machine U is a unitary operation on $\mathbb{C}^2 \otimes \mathbb{C}^2$. This means that at fixed time the system interacts with just a *single* qubit taken out of the bath. In our model we consider that a qubit of the bath undergoes at most one interaction with the system. This assumption is justified by the fact that the bath is assumed to be very large (i.e., “infinite”). Therefore the input state of the ancilla is always ξ , and we write

$$\rho^{(k+1)} = \text{Tr}_B[U(\rho^{(k)} \otimes \xi)U^\dagger] \equiv T_\xi[\rho^{(k)}]. \quad (3)$$

Thermalizing machines.—For the model just introduced, the two requirements I and II read [10]: for all ξ diagonal in the eigenbasis of σ_z ,

$$\text{I: } U_z(\xi \otimes \xi)U_z^\dagger = \xi \otimes \xi, \quad (4)$$

$$\text{II: } \rho^{(n)} = T_\xi^n[\rho] \longrightarrow \xi \quad \forall \rho. \quad (5)$$

The subscript z is meant to remind the reader that we allow the machine U to depend on the eigenbasis of ξ , that is on h . Conversely, we want these requirements to hold for all p , that is for all temperature.

It is important to notice here the existence of an equivalence class. Let $u(x) = P_0 + e^{ix}P_1$, and suppose that U_z satisfies (4) and defines a channel T_ξ . Then $U'_z = (\mathbb{1} \otimes u(\alpha))U_z(\mathbb{1} \otimes u(\beta))$ satisfies (4) as well, and defines the same channel $T'_\xi = T_\xi$. This is easy to see by noticing that $u(x)\xi u(x)^\dagger = \xi$ for all x . This equivalence is a consequence of the freedom of choosing the global phases of $|0\rangle$ and $|1\rangle$ for qubits in the bath. Having noticed this, we can proceed to find all the thermalizing machines.

Take first requirement I: condition (4) implies that the subspaces $P_0 \otimes P_0$, $P_1 \otimes P_1$, and $P_0 \otimes P_1 + P_1 \otimes P_0$ must be invariant under the action of U_z . In fact, on the left-hand side $U_z P_0 \otimes P_0 U_z^\dagger$ appears with the weight p^2 , $U_z(P_0 \otimes P_1 + P_1 \otimes P_0)U_z^\dagger$ with the weight $p(1-p)$, and $U_z P_1 \otimes P_1 U_z^\dagger$ with the weight $(1-p)^2$. Since we want condition (4) to hold for all p , the three subspaces must be separately invariant. This implies $[U_z, H_0] = 0$: the sum of the one-qubit energies is conserved by the interactions. By inspection, one can see that, up to a global phase factor, the most general unitary operations that leave these subspaces invariant is parametrized by five angles; only three of them are left if we choose a suitable representative element in the equivalence class discussed above. Precisely, all unitary operations that fulfill condition (4) can be chosen of the form

$$\begin{aligned} U_z(\phi, \theta, \alpha): & |0\rangle|0\rangle \rightarrow |0\rangle|0\rangle, \\ & |1\rangle|1\rangle \rightarrow |1\rangle|1\rangle, \\ & |0\rangle|1\rangle \rightarrow e^{i(\theta+\alpha)}(c|0\rangle|1\rangle + is|1\rangle|0\rangle), \\ & |1\rangle|0\rangle \rightarrow e^{i(\theta-\alpha)}(c|1\rangle|0\rangle + is|0\rangle|1\rangle), \end{aligned} \quad (6)$$

with $c = \cos\phi$ and $s = \sin\phi$, $\phi \in [0, \frac{\pi}{2}]$, and $\theta, \alpha \in [0, 2\pi]$. We turn now to demonstrate that almost all these machines satisfy condition (5) as well. To do this, let us write the state of the system after n steps as

$$\rho^{(n)} = d^{(n)}P_0 + (1 - d^{(n)})P_1 + k^{(n)}|0\rangle\langle 1| + \text{H.c.} \quad (7)$$

Inserting the explicit form (6) for U_z into (3), we find that the effect of the map T_ξ is given by $d^{(n+1)} = d^{(n)}c^2 + ps^2$ and $k^{(n+1)} = c\lambda k^{(n)}$ with

$$\lambda = e^{i\alpha}(pe^{-i\theta} + qe^{i\theta}). \quad (8)$$

A straightforward iteration gives $d^{(n)}$ and $k^{(n)}$ as a function of parameters $d^{(0)}$ and $k^{(0)}$ of the input state

$$d^{(n)} = [1 - (\cos\phi)^{2n}]p + (\cos\phi)^{2n}d^{(0)}, \quad (9)$$

$$k^{(n)} = k^{(0)}(\lambda \cos\phi)^n. \quad (10)$$

Thus, whenever $\phi \neq 0$, the iteration of T_ξ yields $d^{(n)} \rightarrow p$ and $k^{(n)} \rightarrow 0$ since $|\lambda| \leq 1$; that is, $\rho^{(n)} \rightarrow \xi$: almost all the machines of the form (6) satisfy requirement II as well. In conclusion, the family of thermalizing machines for $h \simeq \sigma_z$ is composed by the $U_z(\phi, \theta, \alpha)$ given by (6) with $\phi \neq 0$ [11].

Dynamical equivalence of machines.—The dynamics (9) of the diagonal term $d^{(n)}$, that is the *dissipation*, is determined only by ϕ . The other parameters θ and α enter only the dynamics (10) of the off-diagonal term $k^{(n)}$, the *decoherence*, through the complex number λ given in (8). Actually, α plays a trivial role: it simply redefines at each iteration the axes x and y in the plane orthogonal to z . Apart from this global rotation, the effect of λ can be visualized as follows: the state of the system undergoes a rotation of $-\theta$ (respectively, $+\theta$) in the (x, y) plane if it interacts with the state $|0\rangle$ (respectively, $|1\rangle$) of the bath, which happens with probability p (respectively, q). This dephasing process contributes only to the decoherence rate. Note also that $|\lambda|$ is unchanged if one replaces θ by $\pi + \theta$. Guided by these considerations, we say that two machines $U_z(\phi, \theta, \alpha)$ and $U_z(\phi, \theta + n\pi, \alpha')$ that differ only on the value of α are *dynamically equivalent*. We choose

$$V_z(\phi, \theta) \equiv U_z(\phi, \theta, 0) = U_z(\phi, \theta, \alpha)[u(\alpha) \otimes u(-\alpha)] \quad (11)$$

as a representative element of the class. The $V_z(\phi, \theta)$ are diagonal in the Bell basis:

$$V_z(\phi, \theta) = P_{00} + P_{11} + e^{i(\theta+\phi)}P_{\Psi^+} + e^{i(\theta-\phi)}P_{\Psi^-}, \quad (12)$$

with $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$. The Hamiltonian representation is easily derived: $V_z(\phi, \theta) = e^{i(\theta/2)}e^{iH(\phi, \theta)}$ with

$$H(\phi, \theta) = \frac{1}{2}[\phi(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) - \theta\sigma_z \otimes \sigma_z]. \quad (13)$$

Finally note that we can handle the dissipation and the dephasing processes separately, since $V_z(\phi, \theta) = V_z(\phi, 0)V_z(0, \theta) = V_z(0, \theta)V_z(\phi, 0)$. By the way, $V_z(\phi, 0)$ is a realization of the two-qubit copying machine, proposed by Niu and Griffiths, that defines Eve's optimal individual attack on the four-state protocol of quantum cryptography [12].

The partial swap.—During the whole construction of the thermalizing machines, we insisted on the fact that the machine may depend on the direction z defined by the local Hamiltonian h . A natural question is whether any of the machines $U_z(\phi, \theta, \alpha)$ is actually independent of z : such a machine would thermalize the state of the system for all one-qubit Hamiltonians $h = -E\hat{n} \cdot \vec{\sigma}$. It turns out [13] that there exists a unique machine with this property, which is $V(\phi, -\phi)$. This machine is a *partial swap*, since

$$V(\phi, -\phi) = e^{-i\phi}(\cos\phi\mathbb{1} + i\sin\phi U_{sw}), \quad (14)$$

where $U_{sw} = V(\frac{\pi}{2}, -\frac{\pi}{2})$ is the swap operation, i.e., it is the unitary operation whose action is $|\psi_1\rangle \otimes |\psi_2\rangle \rightarrow |\psi_2\rangle \otimes |\psi_1\rangle$ for all $|\psi_1\rangle, |\psi_2\rangle \in \mathbb{C}^2$. The partial swap conveys the intuitive idea, that at each collision part of the information contained in the state of the system is transferred into the bath. This machine is the cornerstone of the quantum-information process called *homogenization* [13]. For the dissipation, i.e., apart from phase fluctuations, all thermalizing machines are equivalent to the partial swap: $V(\phi, \theta) = V(0, \theta + \phi)V(\phi, -\phi)$.

This concludes the characterization of the family of the thermalizing machines. In the remainder of the paper, we study their properties, first in terms of thermodynamics, then from the standpoint of quantum information.

Relaxation times.—We would like to pass from the discrete dynamics indexed by n to a continuous-time dynamics with parameter t . To perform the limit, we set $n = t/\tau_0$, and we let the interaction time τ_0 go to zero together with ϕ and θ , keeping constant the dissipation rate $\frac{\phi^2}{\tau_0} = \frac{1}{T_1}$ and the phase fluctuation rate $\frac{2\theta^2}{\tau_0} = \frac{1}{T_{pf}}$. We have $(\cos^2\phi)^n \approx (1 - \phi^2)^{t/\tau_0} \rightarrow e^{-t/T_1}$, and $(|\lambda|\cos\phi)^n \approx [(1 - 2pq\theta^2)(1 - \frac{\phi^2}{2})]^{t/\tau_0} \rightarrow e^{-t/T_2}$ with

$$\frac{1}{T_2} = \frac{1}{2T_1} + pq\frac{1}{T_{pf}} = \frac{1}{2T_1} \left(1 + 4pq \lim_{\tau_0 \rightarrow 0} \frac{\theta^2}{\phi^2}\right). \quad (15)$$

Thus in the continuous-time limit, the processes of dissipation (9) and decoherence (10) are exactly exponential:

$$d(t) = e^{-t/T_1}d(0) + (1 - e^{-t/T_1})p, \quad (16)$$

$$|k|(t) = e^{-t/T_2}|k|(0), \quad (17)$$

with the relaxation times T_1 and T_2 defined in the usual way [14]. For $\theta = 0$ or at zero temperature, the bound $T_1 \geq \frac{1}{2}T_2$ (see, e.g., [6], p. 120) is saturated.

Fluctuation-dissipation (FD) theorem.—A FD theorem links the fluctuations at equilibrium and the mechanisms

of dissipation. Usually, this link is derived in a different framework [7]: in particular, a continuous spectral density of the bath is normally assumed, while here H_B exhibits finite gaps. Nevertheless, one can define a measurable quantity associated to fluctuations and dissipation. Consider the following protocol. First, the system is prepared in the equilibrium state ξ and is measured in the basis of its eigenstates P_0 and P_1 . Obviously, the mean values of one-qubit observables A are unaffected by this measurement. Then we let the system undergo n interactions with the bath qubits: from the state P_j ($j = 0, 1$) in which it had been found by the measurement, the system evolves into the state $\rho_j^{(n)} = T_\xi^n[P_j] = (1 - c^{2n})\xi + c^{2n}P_j$ according to (9). By the definition of equilibrium, $p\rho_0^{(n)} + q\rho_1^{(n)} = \xi$; in particular, the mean value of A holds unchanged. However, due to the information gained through the measurement, now we have also access to the following statistical quantity:

$$F_A^{(n)} = \sqrt{p[\text{Tr}(\delta_0^{(n)}A)]^2 + q[\text{Tr}(\delta_1^{(n)}A)]^2}, \quad (18)$$

where $\delta_j^{(n)} = \rho_j^{(n)} - P_j$ is the deviation from the measured state P_j after n interactions. $F_A^{(n)}$ is a measure of the fluctuations of A ; the dissipative element can be seen through the fact that, if $F_A^{(n)} \neq 0$, then the fluctuations have partly erased the information that we had obtained through the measurement. Writing $D^{(n)} = [1 - (\cos\phi)^{2n}]$ we find

$$F_A^{(n)} = D^{(n)} \frac{1}{2 \cosh(\beta E)} |\text{Tr}(A\sigma_z)|. \quad (19)$$

In the continuous time limit, $D^{(n)}$ is replaced by $D(t) = (1 - e^{-t/T_1})$. This is our FD theorem: the fluctuations F are proportional to the dissipation D through a function of the temperature. The fluctuations are absent at zero temperature, while they are maximal at infinite temperature. Usually one considers the fluctuations of the one-qubit Hamiltonian h , in which case $|\text{Tr}(h\sigma_z)| = 2E$ the splitting of the energy levels.

We proceed now to discuss the link between dissipation and entanglement under two complementary standpoints (a third approach is given in Ref. [13]). The last equality in (11) means that $U_z(\phi, \theta, \alpha)$ is equivalent to $V_z(\phi, \theta)$ up to local unitaries (LU); thus we can restrict to the $V_z(\phi, \theta)$ for the study of entanglement.

Dissipation and entangling power.—The entangling power of a unitary operation U has been given different definitions [15–17]. Here, we are interested in the creation of entanglement during the thermalization process. In this context, the natural definition of the entangling power of a thermalizing machine $V = V_z(\phi, \theta)$ is

$$\mathcal{E}[V] = \max_p \mathcal{E}(V\rho \otimes \xi V^\dagger), \quad (20)$$

with $\mathcal{E}(\cdot)$ a measure of entanglement. As we said above, for two qubits there exists a measure of entanglement C , called *concurrence*, that is computable, basically by ranking the eigenvalues of a 4×4 matrix [9]. This may be a

tedious task on the paper, but is a trivial one for a computer. Performing the optimization, we find for $p \geq q$

$$C[V_z(\phi, \theta)] = C(VP_1 \otimes \xi V^\dagger) = p \sin 2\phi. \quad (21)$$

The maximal entanglement is thus produced when the input state is the excited state $|1\rangle$. The phases fluctuations, measured by θ , do not show up: the entangling power of $V_z(\phi, \theta)$ depends only on the dissipation, measured by ϕ . Moreover, if we want to introduce small fluctuations into the bath [10] (and *a fortiori* in the continuous-time limit), we must consider small values of ϕ . In this limit, the entangling power is increasing with dissipation.

Equivalence under LU.—We have noticed above that $U_z(\phi, \theta, \alpha)$ is LU equivalent to $V_z(\phi, \theta)$. This is a particular case of a general theorem [16] stating that any unitary operation on two qubits is LU equivalent to $U_d = e^{iH_d}$, where $H_d = \sum_{i=x,y,z} \mu_i \sigma_i \otimes \sigma_i$. In our case $\mu_x = \mu_y = \frac{\phi}{2} \in [0, \frac{\pi}{4}]$; and $\mu_z = -\frac{\theta}{2}$. Since $V_z(\phi, \pi + \theta) = [\sigma_z \otimes \sigma_z] V_z(\phi, \theta)$, one can always choose $\theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ within LU equivalence. Now, for parameters in these ranges, the μ_i are uniquely determined [18]. Therefore $U_z(\phi, \theta, \alpha)$ is LU equivalent to $V_z(\phi', \theta')$ if and only if $\phi = \phi' \in [0, \frac{\pi}{2}]$ and $\theta' = \theta \bmod \pi$. In conclusion, two thermalizing machines are LU equivalent if and only if they are dynamically equivalent.

Irreversibility.—We conclude on some general considerations about irreversibility. The thermalization process that we described is certainly reversible, since it involves only unitary operations. Thermalization appears as a consequence of entanglement, not of measurements. The environment does not play the role of measuring apparatus, but of “waste basket for information.” In fact, the information encoded in the initial state of the system ρ is not lost after the thermalization process, but is encoded in a different way, being spread between the system and the bath. The initial state of the system can be reconstructed only if one knows which qubits of the bath have interacted with the system, and in which order. Without this knowledge, any attempt of reconstruction of the initial state will fail [13]. Thus, irreversibility arises here as the interplay of two information processes: (i) the *quantum information* on the initial state of the system is spread between the system and the bath, still in a reversible way; (ii) the *classical information* about the order of the collisions is lost, leading to the practical impossibility of running the process backwards. As an application, one can define “safes” for quantum information that can be “opened” with classical keys [13].

In summary, we have discussed the family of the thermalizing machines for two qubits. These unitary operations can be decomposed into two processes, dissipation and decoherence. Dissipation is linked to fluctuations—and this is expected, although our FD theorem is derived in a different framework than usual—and to

the entangling power of the machine in the process. Both dissipation and decoherence are related to equivalence under local unitaries.

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