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DOI: 10.1103/PhysRevLett.88.097905
Thermalizing Quantum Machines: Dissipation and Entanglement

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(Received 16 October 2001; published 19 February 2002)

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Citation: Physical Review Letters 88, 097905-1 (2002); doi: 10.1103/PhysRevLett.88.097905

PACS numbers: 03.67.–a, 03.65.Ud, 03.65.Yz, 05.70.Ln

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. For entanglement, we give the family of all the thermalizing machines acting on two qubits, and a fluctuation-dissipation theorem for the thermalizing channel that these 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 of qubits. The free Hamiltonian for the whole system is

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

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 \( \xi = e^{-\beta h}/\text{Tr}(e^{-\beta h}) = \frac{1}{\beta} [1 + \tanh(\beta E) \sigma_z] \), 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 \( \sigma_z \); thus

\[ \rho_{\text{in}} = \text{Tr}_B(\rho_S \otimes \rho_B). \]

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.

\[ \rho_{\text{out}} = \text{Tr}_B(\rho_U \otimes \rho_B). \]
\[ \xi = pP_0 + qP_1, \quad q = 1 - p, \]  
(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 \( \xi \), and we write

\[ \rho^{(k+1)} = T_{\xi}[\rho^{(k)}]. \]  
(3)

**Thermalizing machines.**—For the model just introduced, the two requirements I and II read [10]: for all \( \xi \) diagonal in the eigenbasis of \( \sigma_z \),

\begin{align*}
\text{I:} & \quad U_z(\xi \otimes \xi)U_z^\dagger = \xi \otimes \xi, \quad (4) \\
\text{II:} & \quad \rho^{(n)} = T_{\xi}^n[\rho] \longrightarrow \xi \quad \forall \rho. \quad (5)
\end{align*}

The subscript \( z \) is meant to remind the reader that we allow the machine \( U \) to depend on the eigenbasis of \( \xi \), 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 \( u(x) = P_0 + e^{i\phi}P_1, \) and suppose that \( U_z \) satisfies (4) and defines a channel \( T_{\xi} \). Then \( U_z^\dagger = (\mathbb{I} \otimes u(x))U_z(\mathbb{I} \otimes u(\beta)) \) satisfies (4) as well, and defines the same channel \( T_{\xi}^\dagger = T_{\xi} \). 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 \( U_z(\mathbb{I} \otimes P_0)U_z^\dagger \) 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 \( U_z(U_1 \otimes P_1 + U_0 \otimes P_0)U_z^\dagger \) 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 \( U_z(\phi, \theta, \alpha): |0\rangle\langle 0| \rightarrow |0\rangle\langle 0|, \) \[ |1\rangle\langle 1| \rightarrow |1\rangle\langle 1|, \]  
(6)

\[ |0\rangle\langle 0| \rightarrow e^{i(\theta + \alpha)}(c|0\rangle\langle 1| + is|1\rangle\langle 0|), \]  
\[ |1\rangle\langle 0| \rightarrow e^{i(\theta - \alpha)}(c|1\rangle\langle 0| + is|0\rangle\langle 1|), \]  
with \( c = \cos \phi \) and \( s = \sin \phi \), \( \phi \in [0, \frac{\pi}{4}], \) 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

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

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

\[ \lambda = e^{i\alpha}(\cos \phi) e^{-i\theta} + q e^{i\theta}. \]  
(8)

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

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

\[ k^{(n)} = k^{(0)}(\lambda \cos \phi)^n. \]  
(10)

Thus, whenever \( \phi \neq 0 \), the iteration of \( T_{\xi} \) yields \( d^{(n)} \to p \) and \( k^{(n)} \to 0 \) since \( |A| \leq 1 \); that is, \( \rho^{(n)} \to \xi \); almost all the machines of the form (6) satisfy requirement II as well. In conclusion, the family of thermalizing machines for \( h = \sigma_z \) 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 \( \phi \). The other parameters \( \theta \) and \( \alpha \) enter only the dynamics (10) of the off-diagonal term \( k^{(n)} \), the decoherence, through the complex number \( \lambda \) given in (8). Actually, \( \alpha \) 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 \( \lambda \) 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 \( |A| \) is unchanged if one replaces \( \theta \) 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 \( \alpha \) are dynamically equivalent. We choose

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

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

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

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

\[ H(\phi, \theta) = \frac{1}{2} [\phi(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y - \theta \sigma_z \otimes \sigma_z)], \]  
(13)
Finally note that we can handle the dissipation and the dephasing processes separately, since \( V_z(\phi, \theta) = V_z(\phi, \theta) V_z(0, \theta) = V_z(0, \theta) V_z(\phi, 0) \). 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 \( h = -E\vec{n} \cdot \vec{\sigma} \). 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

\[
V(\phi, -\phi) = e^{-i\phi} (\cos \phi 1 + i \sin \phi U_{sw}),
\]

where \( U_{sw} = V(T, -\pi T) \) is the swap operation, i.e., it is the unitary operation whose action is \( |\psi_1\rangle \otimes |\psi_2\rangle \to |\psi_2\rangle \otimes |\psi_1\rangle \) 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 \( \tau_0 \) go to zero together with \( \phi \) and \( \theta \), keeping constant the dissipation rate \( \frac{\phi^2}{\tau_0} = \frac{1}{\tau_1} \) and the phase fluctuation rate \( \frac{\phi^2}{\tau_0} = \frac{1}{\tau_2} \). We have \( \cos^2 \phi^n = (1 - \phi^2)^{1/\tau_0} \to e^{-t/\tau_1} \), and \( (|\lambda| \cos \phi)^n = \left[(1 - 2pq\theta^2)/1 - \phi^2\right]^{1/\tau_0} \to e^{-t/\tau_2} \) with

\[
\frac{1}{T_2} = \frac{1}{2T_1} + \frac{pq}{1 - \phi^2},
\]

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

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

\[
|\lambda|(t) = e^{-t/T_2} |\lambda|(0), \quad (17)
\]

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 \( \xi \) 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 \( \rho_j^{(n)} = T_0^{(n)} [P_j] = (1 - c^{2n}) \xi + c^{2n} P_j \) according to (9). By the definition of equilibrium, \( p P_0^{(n)} + q P_1^{(n)} = \xi \); 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:

\[
F_A^{(n)} = \frac{1}{2} \left[ p \left[ \text{Tr}(\delta_0^{(n)} A) \right]^2 + q \left[ \text{Tr}(\delta_1^{(n)} A) \right]^2 \right],
\]

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

\[
F_A^{(n)} = D^{(n)} \frac{1}{2 \cosh(\beta E) \left[ \text{Tr}(A \sigma_z) \right]}. \quad (19)
\]

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

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

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 \( 4 \times 4 \) 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 $p \geq q$

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

The maximal entanglement is thus produced when the input state is the excited state $|1\rangle$. The phases fluctuations, measured by $\theta$, do not show up: the entangling power of $V_z(\phi, \theta)$ depends only on the dissipation, measured by $\phi$. 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 $\phi$. 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 $H_d = \sum_{x,y,z} \mu_x \sigma_x \otimes \sigma_y$. In our case $\mu_x = \mu_y = \frac{\phi}{\pi} \in [0, \frac{\pi}{2}]$; and $\mu_z = -\frac{\pi}{2}$. Since $V_z(\phi, \pi + \theta) = [\sigma_x \otimes \sigma_y]V_z(\phi, \theta)$, one can always choose $\theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ within LU equivalence. Now, for parameters in these ranges, the $\mu_i$ 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 $\theta' = \theta \mod \pi$. 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 $\rho$ 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.

We acknowledge fruitful discussions with Ignacio Cirac, Günther Mahler, and Sandu Popescu. Part of this work was prepared during the ESF Conference on Quantum Information (Gdańsk, 10–18 July 2001). This work was partially supported by the European Union project EQUIP (IST-1999-11053).

[5] We do not discuss the question of how the bath reached the equilibrium state. It is believed that QM should ultimately answer also this question; see Ref. [1].
[10] The second part of requirement II, namely the fact that the partial state of the bath must not undergo important changes, will be met in the physical discussion by requiring that the interactions are weak.
[11] In the case $\cos \phi = 1$, we have $d^{(n)} = d^{(0)}$ for all $n$, but still $k^{(n)} \rightarrow 0$, unless $|\alpha| = 1$, i.e., unless $\theta = 0$. So $\rho^{(n)} \rightarrow dP_0 + (1 - d)P_0$; the iteration of $T_\xi$ does not converge to the state of the bath $\xi$, but is a pure decoherence process.
[18] This uniqueness is stated in W. Dür et al., quant-ph/0112124, that refers for the demonstration to a paper in preparation. In this paper, the ranges for the parameters are given in a different way, which is found to be equivalent by direct inspection.