Thermodynamic cost of reversible computing
Lev B. Levitin and Tommaso Toffoli

Since reversible computing requires preservation of all information throughout the entire computational process, this implies that all errors that appear as a result of the interaction of the information-carrying system with uncontrolled degrees of freedom must be corrected. But this can only be done at the expense of an increase in the entropy of the environment corresponding to the dissipation, in the form of heat, of the "noisy" part of the system’s energy.

This paper gives an expression of that energy in terms of the effective noise temperature, and analyzes the relationship between the energy dissipation rate and the rate of computation. Finally, a generalized Clausius principle based on the concept of effective temperature is presented.

1 Cost of computing in the presence of noise

The concept of reversible computing was introduced in [1, 11, 3] with the idea to get rid of the immense energy dissipation and heat generation caused by the irreversibility of conventional computing processes. In general, logical reversibility in computation is a necessary but not sufficient condition for physical reversibility. However, in quantum computing these two characteristics come together: any violation of physical reversibility of the evolution of the controlled information-carrying degrees of freedom represents noise that, if left unchecked, will destroy the computation. Thus, it is natural to consider the problem of reversible computing in a quantum milieu.

Reversible computing is by its nature closer to communication than to conventional computing, and therefore it calls for being analyzed from the information-theoretical standpoint. Indeed, if it is true that “communication is computation of the identity function,” then reversible computation is computation of a bijective function: there is a one-to-one correspondence between the set of all possible input data and that of all possible results of the specified computation. Paradoxically, not only does this requirement make the physical implementation of reversible computation more difficult, but it also creates a specific cause of energy dissipation and increase of the entropy of the environment.

Indeed, while at every stage of a conventional computing process we are only concerned with the integrity of that part of the information that is going to contribute to the final result (usually, a small fraction of the information presented in the input data), the precondition of reversible computing is preservation of all information included in the choice of the initial conditions for any particular instance of computation throughout the the entire process of computing. However, this goal cannot be achieved for free. The state of the information-carrying system (the controlled degrees of freedom) is subject to noise owing to two factors: the statistical nature of the interaction between the system and the external devices implementing the required transformation of the system state, and the interactions with uncontrolled degrees of freedom (the environment). As a result, errors appear in the state of the system, which requires corrections that inevitably lead to energy dissipation, i.e., to an increase of the entropy of the environment.

Henceforth we call ‘system’ the collection of controlled degrees of freedom involved in the process of computation, rather than the entire physical object.

Suppose that we start with an ensemble \( \{ \rho_0^i, p_i \} \) of orthogonal, pure initial states, described by density matrices \( \rho_0^i \) that occur with probabilities \( p_i \). Then the initial information \( I_0 \) (i.e., the information in the ensemble of the chosen states \( \rho_0^i \)) about the ensemble of the initial data labeled by \( i \) is given by

\[
I_0 = - \sum_i p_i \ln p_i = - \text{Tr} \rho^0 \ln \rho^0,
\]

where \( \rho^0 = \sum_i p_i \rho_0^i \) is the a priori density matrix of the ensemble. The entropy of each initial state is zero. After performing a step of the computational process (such as, e.g., application of a “quantum gate”), we obtain an ensemble \( \{ \rho_i, p_i \} \), where the density matrices \( \rho_i \) are in general neither pure nor orthogonal. Note that, in general, matrices \( \rho_i \) may describe states of a different physical system than the states characterized by \( \rho_0^i \). What is important, however, is that there exists a one-to-one correspondence between the sets \( \{ \rho_0^i \} \) and \( \{ \rho_i \} \).

The average entropy \( \overline{H} \) of the state after the computation step is

\[
\overline{H} = - \sum_i p_i \text{Tr} \rho_i \ln \rho_i > 0.
\]

Now the information \( I \) conveyed by the state ensemble about the initial state is

\[
I \leq H - \overline{H} \leq I_0, \quad (1)
\]

where

\[
H = - \text{Tr} \rho \ln \rho, \quad \text{with} \quad \rho = \sum_i p_i \rho_i.
\]

Inequality (1) follows from the entropy defect principle [4].

In order to achieve reversibility, the initial ensemble of states should possess sufficient redundancy to turn inequality (1) into an equality, or, in other words, to make \( I = I_0 \). Then the output state \( \rho_0 \) uniquely determines the corresponding input state \( \rho_0^i \). The reversibility condition allows us to consider a “reverse channel” with ensembles \( \{ \rho_i, p_i \} \) as input and \( \{ \rho_0^i, p_i \} \) as output. In this channel, the quantity \( \overline{H} \) plays the role of equivocation [10]. It expresses the effect of noise and the presence of errors in the results of the computation. According to Shannon’s 10th theorem (the
“correction channel theorem” [10], \( \mathcal{H} \) is equal to the minimum additional information required in order to correct all the errors in the state of the system and thereby preserve the initial amount of information (though, in general, in a transformed form). In other words, to correct the errors, the entropy of the information-carrying system must be decreased by the value of \( \mathcal{H} \). Of course, this can be done only at the price of an entropy increase of at least \( \mathcal{H} \) in other degrees of freedom (e.g., the environment). The actual amount of energy that has been dissipated within the system depends on the concrete properties of the system itself, as shown by the following considerations (cf. [5]):

Denote by \( E(T') \) the energy of the system in the state of thermal equilibrium at temperature \( T' \). The increase of the average entropy \( \mathcal{H} \) means that part of the energy has been transformed into heat in the system or transferred to the system in the form of heat. How large is this part? It is equal to the energy \( E(T) \) that the system would have had in the state of thermal equilibrium at temperature \( T \), where \( T \) is determined by the value \( \mathcal{H} \) of entropy increase according to the relation

\[
\mathcal{H} = H(T) = \int_0^T \frac{1}{kT'} \frac{dE(T')}{dT'} dT';
\]

thus, \( T \) has the meaning of an effective noise temperature.

The concept of effective noise temperature was first introduced in [5]. Being applicable to any non-equilibrium state of a system, the effective temperature has, nevertheless, the same fundamental properties as the usual temperature in the thermodynamics of equilibrium systems (and coincides with latter at equilibrium). In particular, it can be shown that if two non-equilibrium physical systems have effective temperatures \( T_1 \) and \( T_2 \), where \( T_1 < T_2 \), and corresponding “thermal” energies \( E_1(T_1) \) and \( E_2(T_2) \) as defined by (2), it is impossible to transfer an amount of energy \( \Delta E \) from the first system to the second by decreasing \( E_1(T_1) \) by an amount \( \Delta E \) and correspondingly increasing \( E_2(T_2) \) by the same or a smaller amount as a sole result of a physical process. In fact, this property represents a generalized Clausius principle[2]. One is thus justified in regarding \( E(T) \) as an amount of energy converted into heat.

In the absence of noise (\( \mathcal{H} = 0 \)), after one step the system will find itself in the pure state corresponding to the initial state \( \psi_0 \). If \( \mathcal{H} \neq 0 \), this implies a nonzero probability of being in a state different from the correct one—the probability of error. Correspondingly, in the calculation of \( E(T) \), if \( \mathcal{H} = 0 \), then \( T = 0 \) and \( E(T) = 0 \), as if the system were in its ground state. If \( \mathcal{H} \neq 0 \), then \( T \neq 0 \) and \( E(T) \neq 0 \). \( E(T) \) can be expressed alternatively as a function of the entropy \( \mathcal{H} \), or of the probability of being in a non-ground state—which we interpret below as the probability of error.

It follows from the above considerations that the procedure of error correction entails removing an amount of heat \( E(T) \) from the system and applying to it an amount of work required to restore the correct state.

Even though it arises from disturbances introduced into a system by interactions with its environment, the noise temperature is not equal, in general, to the temperature of the environment itself (were the latter at thermal equilibrium).

Note that the minimum amount of heat \( Q_e \) to be ultimately transferred at every step to an environment at temperature \( T_e \) (an “infinite, constant-temperature heat sink”) to ensure continuous, closed-cycle operation of the invertible computing machinery envisaged here is not equal, in general, to \( E(T) \). In fact, in a reversible process, \( Q_e = \mathcal{H}T_e \). Indeed, if \( T_e < E(T)/\mathcal{H} \) we could even produce some “useful work” by removing heat \( E(T) \) from our system. However, in a real situation, usually \( T_e \geq E(T)/\mathcal{H} \) (we cannot allow the computing system to “heat up” too much since too large a probability of error would make the state of the system incorrectible) and thus \( Q_e \geq E(T) \).

One could reason that the amount of dissipated energy can be made arbitrarily small if one works with “low energy” states. But it should be borne in mind that the lower the energy, the larger the time taken by each computational step. As shown in [3] [7] [10], the minimum time for transforming a state to an orthogonal state (“flipping a qubit”) is

\[
\tau \geq \frac{h}{4E},
\]

where \( h \) is Planck’s constant and \( E \) the average energy of the system. This inequality turns into an equality only for a system with two orthogonal states. For a sequence of \( N \) mutually orthogonal states a stronger inequality,

\[
\tau \geq \frac{N - 1}{N} \frac{h}{2E},
\]

becomes valid[8]. Thus, the maximum rate of computation, i.e., the number \( R \) of computational steps per unit time is proportional to the quantum-mechanical average energy of the system, that is,

\[
R = \frac{4E}{h} \quad \text{for two orthogonal states and}
\]

\[
R = \frac{N}{N - 1} \frac{2E}{h} \quad \text{for a sequence of } N \text{ such states.}
\]

As shown below, it follows from [2], [3], and [10] that, the faster one wants to perform a computation, the more energy per step will be dissipated in the form of heat. The energy dissipation per computational step is then expressed as an increasing function of both the noise temperature and the rate of computation (i.e., the number of computational steps per unit time).

2 Examples

We shall consider first two representative examples.

Example 1. The qubit.

Let a system with two orthogonal states (a two-dimensional Hilbert space) have two energy levels, \( E_0 = 0 \) and \( E_1 \). The maximum rate of computation is achieved for two pure states \( \psi_1 = \frac{1}{\sqrt{2}}(|E_0\rangle + |E_1\rangle) \) and \( \psi_2 = \frac{1}{\sqrt{2}}(|E_0\rangle - |E_1\rangle) \), with quantum-mechanical average energy \( E = E_1/2 \) (cf. [8]), which turn into one another at each
computational step. Their density matrices in the stationary basis \( \{ |E_0 \rangle, |E_1 \rangle \} \) are

\[
\varrho^0_1 = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} \quad \text{and} \quad \varrho^0_2 = \begin{bmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{bmatrix}.
\]

In this case

\[
R = \frac{4E}{\hbar} = \frac{2E_1}{\hbar}.
\]

Suppose now that there is a probability \( \varepsilon \) of error, so that the resulting states are each a mixture of the correct state with probability \( 1 - \varepsilon \) and the other with probability \( \varepsilon \), with density matrices

\[
\varrho_1 = \begin{bmatrix} 1/2 & 1/2 - \varepsilon \\ 1/2 - \varepsilon & 1/2 \end{bmatrix}, \quad \varrho_2 = \begin{bmatrix} 1/2 & -1/2 + \varepsilon \\ -1/2 + \varepsilon & 1/2 \end{bmatrix}.
\]

The average entropy of the states is

\[
H = -\varepsilon \ln \varepsilon - (1 - \varepsilon) \ln(1 - \varepsilon),
\]

and is equal to the entropy of a thermal equilibrium state with temperature \( T \) described by the density matrix

\[
\varrho_\text{eq} = \begin{bmatrix} 1 - \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}, \quad \varepsilon = \frac{e^{-E_1/kT}}{1 + e^{-E_1/kT}}.
\]

The states in (6) are thermodynamically equivalent, since they have the same entropy \( H \). In particular, they can be represented by mixtures of the pure state \( |1/2 \rangle \langle 0 | \) with the same coefficients, respectively, \( 1 - 2\varepsilon \) and \( 2\varepsilon \):

\[
\varrho_i = (1 - 2\varepsilon) \begin{bmatrix} 1/2 & \pm 1/2 \\ \pm 1/2 & 1/2 \end{bmatrix} + 2\varepsilon \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}, \quad i = 1, 2;
\]

\[
\varrho_\text{eq} = (1 - 2\varepsilon) \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + 2\varepsilon \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}.
\]

Thus, \( T \) in (7) is the effective noise temperature as defined by (2).

The energy of the system at the thermal equilibrium state with temperature \( T \) is

\[
E(T) = \frac{e^{-E_1/kT}}{1 + e^{-E_1/kT}} E_1.
\]

Hence, from (5) and (3),

\[
E(T) = \frac{e^{-hR/2kT}}{1 + e^{-hR/2kT}} \frac{hR}{2},
\]

and thus, by (7),

\[
E(T) = \frac{hR}{2} \varepsilon.
\]

The quantity \( E(T) \) represents the lower bound on energy dissipation per step of computation—in other words, per “flipping of the qubit.” Thus, for a qubit, assuming a fixed probability of error, the minimum energy dissipation is proportional to the rate of computation. Consequently, the amount of heat \( Q \) generated per unit of time is proportional to the square of the rate of computation:

\[
Q = \frac{hR^2}{2} \varepsilon.
\]

**Example 2. Quantum harmonic oscillator.**

A sequence of \( N \) orthogonal non-stationary states of a quantum harmonic oscillator consists of wavefunctions

\[
\psi_m = \sum_{n=0}^{N-1} \frac{1}{\sqrt{N}} e^{-2i\pi mn/N} |E_n\rangle, \quad m,n=0,1,\ldots,N-1,
\]

where \( |E_n\rangle \) is the stationary state with energy \( E_n = n\Delta E \) and \( \Delta E \) is the separation of the energy levels (the ground-state energy is taken to be zero). The average energy is \( E = (N-1)\Delta E/2 \).

Sequence (10) provides the maximum rate of computation, given by

\[
R = \frac{2N E}{N - 1} \frac{\hbar}{kT} = N \frac{\Delta E}{\hbar}.
\]

Assume now that, as a result of errors caused by noise, the resulting state is not pure, but has an entropy \( H \). To calculate the part of the energy turned into heat, consider the state of thermal equilibrium with the same entropy. The energy corresponding to the thermal equilibrium of a harmonic oscillator at temperature \( T \) is

\[
E(T) = \frac{\Delta E}{e^{\Delta E/kT} - 1}.
\]

Hence, for a given maximum computation rate, the energy dissipation per computational step is

\[
E(T) = \frac{hR/N}{e^{hR/(NkT)} - 1}.
\]

The error probability (the total probability to be in a state which is orthogonal to the correct one) is in this case

\[
\varepsilon = e^{-\Delta E/kT} = e^{-hR/(NkT)}.
\]

Hence, in terms of error probability,

\[
E(T) = \frac{\varepsilon hR}{1 - \varepsilon N}.
\]

Thus, the rate of energy dissipation (i.e., heat production per unit time) is

\[
Q = \frac{\varepsilon hR^2}{1 - \varepsilon N}.
\]

Through expressions (9) and (11), the above two examples suggest a general conjecture—that for a fixed error probability (i.e., for a given intensity of noise effects) the energy dissipation rate increases quadratically with the rate of computation.

In the next section we shall confirm this conjecture in the limiting case of a large number of degrees of freedom.

**3 General case: a system with many degrees of freedom**

The exact form of the expression for heat production depends on the specific details of the computing system’s energy-level structure. Nevertheless, under rather general
assumptions, a closed-form result can be obtained for a broad class of systems.

Following the analysis given in [8], let’s consider a system with many degrees of freedom that runs through a long sequence (\(N \gg 1\)) of mutually orthogonal states. It is shown in [8] Sect. 2.3] that all those states are superpositions of energy eigenstates with all different values of energy,

\[
|\psi_m\rangle = \sum_{n=0}^{N-1} c_n e^{-2\pi i E_n / EN} |E_n\rangle,
\]

where

\[
c_n = \sqrt{\frac{E_{n+1} - E_n}{E_N}}
\]

and the average energy \(E\) is asymptotically (\(N \gg 1\))

\[
E = \langle \psi_m | H | \psi_m \rangle = E_N/2.
\]

Let \(T\) be the effective noise temperature of our system. The partition function \(Z\) and the average energy \(E\) of the thermal equilibrium state are

\[
Z = \sum_{n=0}^{\infty} w(E_n) e^{-E_n / kT},
\]

\[
E(T) = \frac{1}{Z} \sum_{n=0}^{\infty} E_n w(E_n) e^{-E_n / kT},
\]

where \(w(E_n)\) is the number of the microstates with energy \(E_n\). For a system with many degrees of freedom one has \(w(E_n) \sim E_n^\alpha\) (for \(n > 0\)), where \(\alpha \geq 1\). Typically [9], \(\alpha \gg 1\). Also, we assume that the zero-energy level is non-degenerate, i.e., \(w(E_0) = 1\).

Let us introduce a dimensionless variable \(x = NE/E_N\) that characterizes the density of the energy levels: the number of energy levels between \(x_n\) and \(x_n + \Delta x\) is equal to \(\Delta x\). Also, suppose that \(w(E_n) = ax_n^\alpha\), where \(a\) is a dimensionless constant. Then expressions (13) and (14) take the following form:

\[
Z = 1 + \sum_{n=0}^{\infty} ax_n^\alpha e^{-(EN/NkT)x_n},
\]

\[
E(T) = \frac{1}{Z} \sum_{n=0}^{\infty} ax_n^{\alpha+1} \frac{E_n}{N} e^{-(EN/NkT)x_n}.
\]

It follows from (11) and (12) that, for \(N \gg 1\), one has \(E_N = hR\). Replacing summation by integration in (15) and (16), we obtain, using Euler’s gamma function \(\Gamma\),

\[
Z = 1 + \int_0^\infty ax^\alpha e^{-(hR/NkT)x} dx
= 1 + a\Gamma(\alpha + 1) \left(\frac{NkT}{hR}\right)^{\alpha+1},
\]

\[
E(T) = \frac{1}{Z} \int_0^\infty ax^{\alpha+1} \frac{hR}{N} e^{-(hR/NkT)x} dx
= \frac{1}{Z} a\Gamma(\alpha + 2) \left(\frac{NkT}{hR}\right)^{\alpha+1}.
\]

It will be convenient to express this result in terms of the error probability \(\varepsilon\), which is equal to the probability to be in a non-ground state, that is,

\[
\varepsilon = 1 - \frac{1}{Z};
\]

then

\[
E(T) = (\alpha + 1)kT \left(1 - \frac{1}{Z}\right) = (\alpha + 1)kT \varepsilon.
\]

Expressing \(kT\) in terms of \(\varepsilon\) from (17), we find that

\[
E(T) = (\alpha + 1)\frac{\varepsilon}{N \left(1 - \varepsilon\right)} \left(\frac{1}{a\Gamma(\alpha + 1)}\right)^{\frac{1}{\varepsilon}} hR.
\]

Thus, the energy dissipation per computational step is proportional to the rate of computation, and so

\[
Q \sim hR^2,
\]

i.e., the rate of heat production is proportional to the square of the computation rate.

**Appendix: A generalized Clausius principle**

**Theorem 1** Given two (in general, non-equilibrium) physical systems with entropies \(H_i\) and \(H_2\), thermal equilibrium functions \(E_1(T)\) and \(E_2(T)\), and effective temperatures \(T_1\) and \(T_2\), defined by equations

\[
H_i = \int_0^{T_i} \frac{1}{kT} dE_i(T) dt, \quad (i = 1, 2)
\]

it is impossible to transfer energy from the first system to the second so as to decrease \(E_1(T_1)\) by an amount of energy \(\Delta E\) and increase \(E_2(T_2)\) by the same or a smaller amount as a sole result of a physical process. We assume that the functions \(E_1, E_2\) that characterize the systems remain unchanged as a result of the process.

**Proof.** Suppose \(E_2(T_2)\) has been decreased by \(\Delta E\) and \(E_2(T_2)\) increased by \(\Delta E' \leq \Delta E\) without any other changes in the environment. As a result, the systems would now have new effective temperatures \(T'_1 < T_1\) and \(T'_2 > T_2\), and corresponding thermal equilibrium energies

\[
E_1(T'_1) = E_1(T_1) - \Delta E,
\]

\[
E_2(T'_2) = E_2(T_2) + \Delta E',
\]

where

\[
\Delta E' = \int_{T'_2}^{T_2} \frac{dE_2(T)}{dT} dT - \Delta E = \int_{T'_1}^{T_1} \frac{dE_1(T)}{dT} dT
\]

(we assume that \(E_1\) and \(E_2\) are monotonically increasing functions). Hence, the total change of entropy would be

\[
\Delta H = \Delta H_1 + \Delta H_2,
\]

where

\[
\Delta H_1 = -\int_{T'_1}^{T_1} \frac{dE_1(T)}{TdT} dT,
\]

\[
\Delta H_2 = \int_{T'_2}^{T_2} \frac{dE_2(T)}{dT} dT.
\]
\[ \Delta H_2 = \int_{T_1}^{T_2} \frac{dE_2(T)}{dT} \, dT. \]

Using the mean value theorem, we get

\[ \Delta H_1 = -\frac{1}{T_1^*} \Delta E, \quad T_1^* < T_1, \quad (20) \]

\[ \Delta H_2 = \frac{1}{T_2^*} \Delta E', \quad T_2 < T_2^*. \quad (21) \]

Obviously, \( T_1^* < T_1 \leq T_2 < T_2^* \).

It follows from (20), (21) that the total change of entropy would be negative:

\[ \Delta H = -\frac{1}{T_1^*} \Delta E + \frac{1}{T_2^*} \Delta E' \leq \frac{T_1^* - T_2^*}{T_1^* T_2^*} \Delta E \leq 0. \]

Thus, such a process is impossible. \( \blacksquare \)

Note that the generalized Clausius principle does not preclude any exchange of work between the two systems, i.e., a process that does not affect the values of \( E_1(T_1) \) and \( E_2(T_2) \).

The significance of these results is that they represent a universal lower bound on the energy dissipation rate in a reversible computation process.

Acknowledgment

The authors are very grateful to Michael Frank (FAMU–FSU) whose deep and thoughtful comments resulted in improvements of this paper and gave us inspiration for future work.

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