

Bachelor´s Thesis

Maxwell Demon in Open Quantum Systems

Iván Pablo Morillas Marco
Physics Degree, UAM

Abstract

This work has studied a functional Maxwell demon in a quantum system formed by quantum dots and electronic reservoirs, used to generate current, and phonons, used for cooling, simulating a quantum Smoluchowski trap. To this end, the density matrix formalism of open quantum systems has been used, thus working with the relevant thermodynamic flows. This is done with the main objective of generating a current in the isothermal regime and with equal chemical potential of the electronic reservoirs. The specific effects of the possible resonances of the system and the range of existence of the demon as a function of its parameters have been analysed.

Contents

1 Introduction to demons	1
1.1 The second law of thermodynamics	1
1.2 The first Maxwell's demons	1
1.3 Do demons work? Smoluchowski, Szilard and Landauer	3
1.4 Demons at the local level	4
2 Quantum systems	4
2.1 Quantum dots and couplings	5
2.2 Capacitive model	6
3 Density matrix formalism in open quantum systems	6
3.1 Time evolution and Liouville–von Neumann equation	6
3.2 Interaction picture and perturbative expansion	7
3.3 Weak-coupling approximations: Born, Markov, and secular	7
3.4 Master equations and stationary regime	9
3.5 Transition rates: Fermi's golden rule	10
3.6 Current and entropy flows	10
4 Autonomous system: conducting DQD with DQD trapdoor (quantum Smoluchowski)	12
4.1 Hamiltonian of the system	13
4.2 Phonon bath	14
4.3 A “small” complication	15
4.4 Why this model?	17
5 Results and discussion	19
5.1 Basic operation and phonon bath	20
5.2 Resonance analysis	22
5.3 Region analysis	24
5.4 A possible alternative	27
6 Conclusions	27

1 Introduction to demons

Description of the quantum dot system, energy discretisation, experiment setup.

1.1 The second law of thermodynamics

The second law of thermodynamics is one of the main pillars of physics. The most traditional forms of this law, such as in the formulations of Clausius and Kelvin, introduce the principle of irreversibility, according to which, in any spontaneous process, the entropy of the system and its environment never decreases. From this, the usual conclusion follows: the entropy of the universe cannot decrease.

‘It is impossible for an autonomous machine, without the aid of any external agent, to transfer heat from one body to another hotter body.’ — Clausius, 1850.

‘It is impossible to construct a device that, using an inert fluid, can produce effective work caused by the cooling of the coldest body available.’ — Kelvin, 1851.

However, these statements are only valid in the macroscopic context, where thermal fluctuations are negligible. In microscopic or nanoscopic systems, these fluctuations cannot be ignored, and a reformulation of the second law is necessary:

“The average entropy cannot decrease when averaged over all possible thermal fluctuations.”

This formulation does not break the second law, but rather recognizes that local and momentary exceptions may exist. One of the theoretical tools that allows quantifying these exceptions is the Evans and Searles fluctuation theorem. This theorem provides a relation for the probability of observing entropy reductions in systems out of equilibrium:

$$P(-\Delta S) = P(\Delta S) \cdot e^{-\Delta S/k_B} \quad (1)$$

Which was obtained after realizing that the ratio between the probabilities of dynamical trajectories in systems out of equilibrium resulted in an exponential factor. When analyzing it, we realize that such a decrease in entropy is possible, but it is exponentially less probable the larger the decrease is, and it implies that for small fluctuations there may be reductions with some frequency, but on average, it continues to increase. In short, this theorem enriches the statistical interpretation of the second law since it shows us that irreversibility really emerges as a statistical phenomenon and, on average, the entropy of the universe continues to grow and it would not be possible to build a perpetual motion machine of the second kind. Not even if this were done at nanoscopic scales.

1.2 The first Maxwell’s demons

The original idea of the demon was first recorded in a letter by Maxwell in 1867, and later formulated in 1871 in his book Theory of Heat. Maxwell’s idea revolved around “making a hole” in the second law with a thought experiment, while it was Kelvin who coined the

term demon due to the capabilities that this system would have in Maxwell's thought experiment.

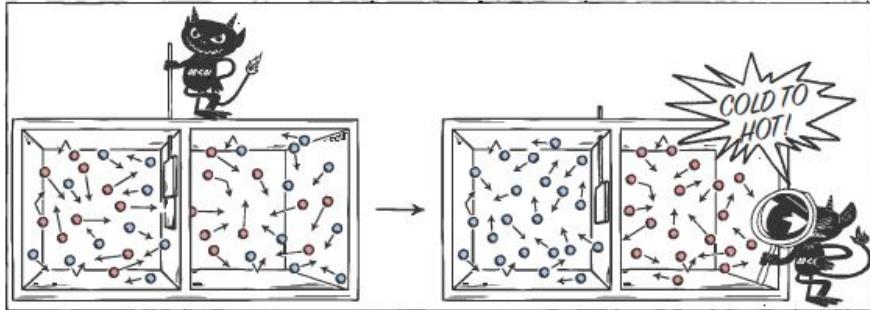


Figure 1: Temperature demon. It opens and closes the door depending on the speed and position of the particle. Image belonging to [5].

First, we will deal with the temperature demon. This consists of an intelligent being that controls a massless and frictionless trapdoor between two chambers or compartments of gas initially isolated in thermal equilibrium. This demon knows the velocities and positions of the particles, in such a way that it can open and close the trapdoor at will according to its interest. In this way, it would move the fast particles to one side and the slow ones to the other, thus providing one colder side and one hotter side without having essentially performed any work. In this way, the entropy of the system would decrease, completely violating the second law of thermodynamics.

In the process, it is important to mention that the demon needs to know or measure the velocity and/or position of the gas molecules in order to know when to open and close the trapdoor. This will be discussed later.

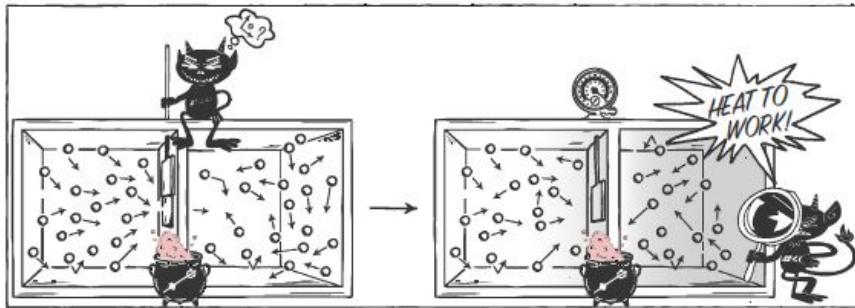


Figure 2: Pressure demon. It simply knows the direction of the particles, opening or closing the door accordingly. Image belonging to [5].

Now looking at the pressure demon, which is a less sophisticated version since it does not know the velocities but only the direction of the motion, it can make the trapdoor move when a particle strikes it in the direction of its interest.

The demon then now works as a directional filter, allowing the particles to accumulate in a first compartment (system side) and blocking the flow from the other compartment; in one they only leave and in the other they only enter.

In this way, a pressure difference is obtained between both compartments, which can be used in mechanical work. In essence, the demon has not influenced the system, so it would be violating the second law.

1.3 Do demons work? Smoluchowski, Szilard and Landauer

Several physicists of the time took Maxwell's proposals and the idea of these two demons seriously, being capable of reducing entropy without performing work and from which perpetual machines could be obtained. Soon, the idea began to be modelled through mechanical devices, such as one-way valves or trapdoors, without the need for observation or demons. It is here where Smoluchowski's studies in 1912 come into play, who developed essential theoretical proposals in this field.

In order to understand what happens with the two previous demons, especially the pressure one, we first introduce Smoluchowski's version of the demon which, anticipating what will be studied later, will be the main inspiration for the analysis of demons in quantum or nanoscopic systems.

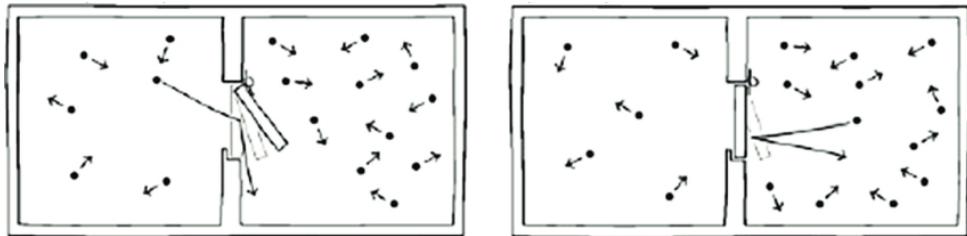


Figure 3: Simple scheme of Smoluchowski's trapdoor. When a particle hits it, it can displace the trapdoor and pass to the other chamber, whereas if it comes from the other side it should bounce. Image belonging to [7].

This version will be called the Smoluchowski trapdoor, which consists of a small light trapdoor that only opens towards one side, so that a particle incident from, for example, the left, can pass through the trapdoor and move to the other side, while, if it arrives from the right, it will collide with the trapdoor, which will close due to the action of a small spring, and will bounce. In this way, in principle, a pressure flow in a single direction is generated that would allow useful work to be extracted from a single thermal reservoir and violate the second law, being a kind of trapdoor equivalent to the pressure demon.

However, we can realize that if we want to replicate this system, the trapdoor cannot but be part of the thermal system; it has its own temperature, a mass at least comparable to that of the particles and thermal fluctuations in the form of Brownian motion. These fluctuations should cause a random component in the opening and closing of the trapdoor and the particles would pass accordingly in both directions, averaging the flow of particles in the system. Basically, that maintained differential pressure would not be generated and useful work could not be continuously extracted: it is not a perpetual motion machine.

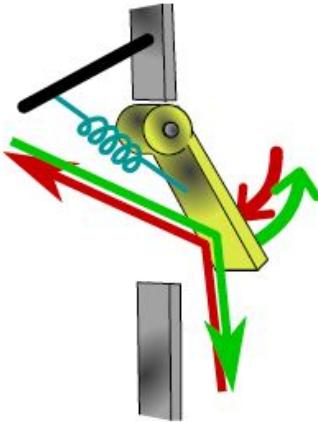


Figure 4: Diagram of the symmetry in Smoluchowski’s trapdoor. Each direction has its inverse, which prevents asymmetry from being generated. Image belonging to [2].

These arguments were presented in a more qualitative and less rigorous way than Feynman would later do, who with his thermal ratchet would end up proving that it is impossible to achieve perpetual motion machines from the random thermal motion of the particles (see appendix). What is true is that, if the trapdoor could somehow be coupled in order to reduce its random motions, it could work. This is what we will analyze in our system later, because quantum systems allow it for us.

In any case, Szilard and Landauer proved that demons cannot violate the second law (see appendix). This is due to the fact that any physical system that performs a measurement of the information of a system, in this case its position, velocity or direction, must have a memory. It is in the act of erasing the memory in order to be able to perform more than one cycle where the erasure of information requires a minimum of energy and (positive) entropy that is greater than or equal to that obtained by the demon.

1.4 Demons at the local level

In this situation it is convenient to ask, how can one proceed? Fortunately, Maxwell’s demons can be very useful, since they can indeed fulfill their task at the local level. Although they do not violate the second law, that does not mean that they do not accomplish the desired effect; the first demon can generate a temperature difference and the second a pressure difference. This decrease in entropy is indeed real at the local level and, ultimately, systems could be generated that, without heat exchange with a thermal bath, can generate work or simply reduce their entropy.

The next step then would be to ask, what happens if we make these demons in a quantum system?

2 Quantum systems

The aim of this work lies in the search and analysis of the possible effects of a Maxwell demon in quantum systems, but what systems are we exactly going to work with? What approximations and models do we apply to them? Before delving into the development of the density matrix formalism, it is convenient to explain this.

2.1 Quantum dots and couplings

Quantum dots (QDs) are nanoscopic structures that confine charge carriers in the three spatial dimensions, generating discrete energy levels like an atom. This property, derived from *quantum confinement*, gives them the name of *artificial atoms*. They are typically fabricated in semiconductor heterostructures such as GaAs/AlGaAs, where metallic gates on a two-dimensional electron gas (2DEG) allow potential regions to be defined and controlled.

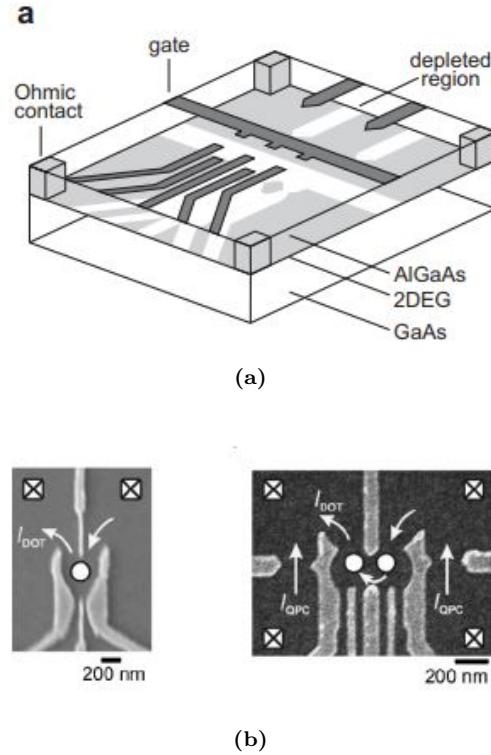


Figure 5: Image belonging to [3]. (a) Three-dimensional scheme of a device based on GaAs/AlGaAs heterostructures that hosts a two-dimensional electron gas (2DEG). Metallic gates on the surface make it possible to define potential regions through electric fields that locally deplete the 2DEG. (b) Electron microscopy of lateral structures: on the left, an electrostatically defined quantum dot; on the right, a double quantum dot system coupled to quantum point contacts (QPCs) for charge detection. The dark regions correspond to areas of 2DEG depleted by the metallic gates.

They exhibit a high controllability (through gate voltages, external couplings or optical pulses) that allows studies in precise engineering of states, coherent transitions and level manipulation. They are ideal in *quantum thermodynamics*, working as engines, rectifiers or Maxwell's demons.

QDs operate as open systems coupled to electronic reservoirs, which allows charge and energy transport, but also exposes them to *decoherence* and dissipation. These effects are modulated through couplings to phonons or losses to the environment.

It is not intended to analyze the detailed experimental setup, but rather to build a theoretical model where the key elements —QDs, reservoirs, coherent and incoherent couplings— allow the functioning of a demon to be studied.

2.2 Capacitive model

With all this, we now connect a hypothetical quantum dot system to a set of reservoirs through tunnel barriers to metallic contacts, which is done with gate electrodes that control the potential of the dot.

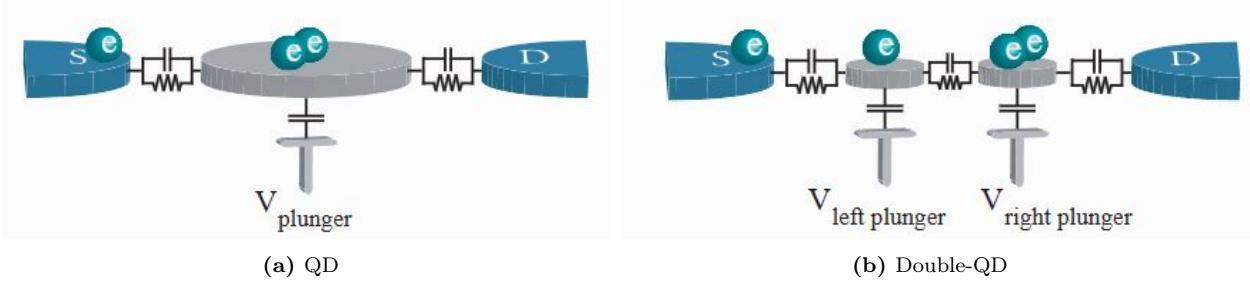


Figure 6: Image belonging to [4]. Scheme of QD (a) and DQD (b) between reservoirs. The energies of each one are modulated with an external potential. This coupling as resistance and capacitance allows tunneling (current flow) and energy blockades.

In this setting, one recognizes a model that describes that the electrostatic interaction energy of the quantum dots is constant, which is very important for our development. We then assume that the interaction between the electrons in the dot and the environment is parametrized by a total capacitance given by the sum of source, gate, and drain:

$$C = C_S + C_D + C_G, \quad (2)$$

Furthermore, we do not make the energy level spectrum depend on the number of electrons. The total energy with N electrons then becomes

$$U(N) = \frac{[-e(N - N_0) + C_S V_S + C_D V_D + C_G V_G]^2}{2C} + \sum_{n=1}^N E_n(B), \quad (3)$$

where N_0 would represent a positive background charge due to the donors of the heterostructure and $E_n(B)$ are the individual energy levels that may depend on an applied magnetic field B .

From this energy, the electrochemical potential is defined as:

$$\mu(N) = U(N) - U(N - 1), \quad (4)$$

This equation leads us to the *Coulomb blockade*, which is very important in our system, and arises when the energetic cost of adding an electron to a quantum dot (QD) is greater than the available thermal energy.

3 Density matrix formalism in open quantum systems

3.1 Time evolution and Liouville–von Neumann equation

We describe the statistical state of a system by the density matrix ρ , which allows us to represent mixtures of quantum states unlike the wave function. In this context, the expectation value of an observable is written as $\langle O \rangle = \text{tr}(\rho O)$, since the density matrix

represents the probabilities of the states in its diagonal and the coherences between them in the off-diagonal terms. For a closed system with Hamiltonian H , the density matrix evolves according to the von Neumann equation, which is a kind of quantum analogue of the classical Liouville equation:

$$\dot{\rho}(t) = -\frac{i}{\hbar} [H, \rho(t)], \quad (5)$$

where $[H, \rho] = H\rho - \rho H$. This unitary dynamics is trace-conserving ($\text{tr}(\rho) = 1$) and keeps ρ positive definite. This time evolution is obtained by applying the time-evolution operator with a time-independent Hamiltonian in the Schrödinger equation. We can define the Liouville superoperator $\mathcal{L}(\rho) \equiv -\frac{i}{\hbar}[H, \rho]$, so that the formal solution is $\rho(t) = e^{\mathcal{L}t}[\rho(0)] = U(t)\rho(0)U(t)^\dagger$ with $U(t) = e^{-iHt/\hbar}$ the unitary evolution.

As in our work, when we deal with an open system, that is, a system S coupled to one or several environments (such as reservoirs R), we focus on the reduced density matrix $\rho_S = \text{tr}_R \rho$, obtained by tracing over the degrees of freedom of the environment. The evolution of this $\rho_S(t)$ is then no longer simply unitary, since the coupling induces dissipation and decoherence. Starting from the total Hamiltonian $H_{\text{tot}} = H_S + H_R + V$ (with V the S - R interaction), the exact equation for $\rho_S(t)$ is generally complicated, as it includes memory (integro-differential). If we now want to derive a time-local master equation for ρ_S , it will be useful to move to the interaction picture.

3.2 Interaction picture and perturbative expansion

Let $H_0 = H_S + H_R$ be the free Hamiltonian (system + environment) and V the interaction. In the interaction picture, operators evolve with H_0 . We define

$$\rho_I(t) = e^{\frac{i}{\hbar}H_0 t} \rho_{SR}(t) e^{-\frac{i}{\hbar}H_0 t} \quad \text{and} \quad V_I(t) = e^{\frac{i}{\hbar}H_0 t} V e^{-\frac{i}{\hbar}H_0 t}. \quad (6)$$

The exact equation of motion in this picture is:

$$\dot{\rho}_I(t) = -\frac{i}{\hbar} [V_I(t), \rho_I(t)], \quad (7)$$

which, upon formal integration, leads us to the Dyson expansion. Assuming that at $t = 0$ the interaction is “switched on”, the perturbative solution up to second order is:

$$\dot{\rho}_I(t) = -\frac{i}{\hbar} [V_I(t), \rho_I(0)] - \frac{1}{\hbar^2} \int_0^t dt' [V_I(t), [V_I(t'), \rho_I(t')]]. \quad (8)$$

The first term (order 1) only contributes if there were initial S - R correlations. For simplicity, we take a factorized initial condition $\rho_{SR}(0) = \rho_S(0) \otimes \rho_R(0)$ (no initial correlation), which cancels that first term. The second term (order 2 in V) reflects processes in which the system interacts twice with the environment. Up to this point we say that the expression is still exact, but to move forward we need physical approximations for V and the environment.

3.3 Weak-coupling approximations: Born, Markov, and secular

In many cases of interest the coupling V is weak compared to the energies that characterize H_S and H_R . This justifies the Born approximation, in which one assumes that

the influence of the system on the environment is negligible to first order; the total state remains approximately given by $\rho_{SR}(t) \approx \rho_S(t) \otimes \rho_R(0)$ during the evolution. This is equivalent to saying that the environment R remains in equilibrium (barely perturbed by S) and that S - R correlations are small of order V^2 . This makes a lot of sense if we simply think of an environment R that is much larger than our system S .

Under this approximation, when taking the trace over R of the previous equation, we can replace $\rho_I(t') \approx \rho_S(t') \otimes \rho_R(0)$ inside the double commutator. The result is a time-local equation of motion for $\rho_S(t)$ with integrals of environment correlation functions. These functions will in general decay over a characteristic time τ_R (the reservoir correlation time).

The next hypothesis is the Markov approximation: we assume that the correlation time of the environment τ_R is sufficiently short compared with the evolution time scales of the system S . Physically, we say that the environment “has no memory” of the perturbations caused by S . Mathematically, the upper limit of the integral is extended to infinity and $\rho_S(t')$ is replaced by $\rho_S(t)$ (since only $t' \approx t$ really matters in the integration). This removes memory of the past and produces a Markovian differential equation for $\rho_S(t)$. After Born and Markov, we obtain approximately:

$$\dot{\rho}_I(t) \approx -\frac{1}{\hbar^2} \int_0^\infty d\tau [V_I(t), [V_I(t-\tau), \rho_I(t)]] , \quad (9)$$

where we have neglected higher-order commutation of t' with respect to t .

Next, we introduce the decomposition $V = \sum_i s_i \otimes r_i$ as a sum of system operators (s_i) and environment operators (r_i). In the interaction picture, $s_i(t)$ and $r_i(t)$ oscillate with H_S and H_R respectively. Substituting this form into the equation and tracing over R , we obtain environment correlations of the type $\langle r_i(t) r_j(t-\tau) \rangle_R$ (bath correlation functions). The Markov approximation implies that these correlations $\langle r_i(t) r_j(t') \rangle$ are only significant for very short $\tau = t - t'$. Therefore, we extend the integration limit to ∞ and assume that $\langle r_i(t) r_j(t') \rangle \rightarrow 0$ for $t - t' > \tau_R$. Likewise, we take $\rho_I(t') \approx \rho_I(t)$ inside the integral.

It is then useful to move to the eigenbasis of H_S . We denote $H_S|m\rangle = E_m|m\rangle$. In this basis, the operators $s_i(t)$ will have components that oscillate with frequencies given by energy differences ($\hbar\omega_{mn} = E_m - E_n$). If we perform the integral in τ (using $\int_0^\infty e^{i\omega\tau} d\tau = \pi\delta(\omega) + i\mathcal{P}(1/\omega)$), we obtain terms proportional to the Dirac delta enforcing energy conservation between system and environment. In fact, the only non-oscillatory (secular) contributions come from resonant terms for which $\omega_{m'n'} = \omega_{nm}$ (equal and opposite energy differences). This assumption is known as the secular or rotating-wave approximation, and it eliminates non-resonant terms that would produce fast oscillations averaging to zero. After this secular approximation, the dynamics of the populations (diagonal elements ρ_{mm}) decouples from that of the coherences ($\rho_{m\neq n}$), and the resulting equation takes a Lindblad form that is completely positive.

Taken together, the main hypotheses to derive the simplified master equation are:

- **Weak coupling (Born):** $\rho_{SR}(t) \approx \rho_S(t) \otimes \rho_R(0)$ holds during the evolution; the environment remains essentially in equilibrium. We retain terms up to second order in V (higher orders are discarded).
- **Memoryless (Markov):** Environment correlations decay rapidly compared with the dynamics of S , so that $\rho_S(t-\tau) \approx \rho_S(t)$ and we extend $\int_0^t \rightarrow \int_0^\infty$.

- **Secular approximation:** If the energy spectrum of S has level spacings that are considerably larger than the dissipative scales, we average non-resonant terms to zero. This guarantees that the reduced density matrix remains positive at all times, eliminating couplings between coherences and populations of different frequencies.

3.4 Master equations and stationary regime

Once the Lindblad-type master equation is specified, it is useful to write the differential equations for each element of the density matrix $\rho_{ij}(t)$ in the eigenbasis of the system $H_S|m\rangle = E_m|m\rangle$. We do not go into the full derivation, as it is very lengthy. These equations naturally separate into equations for the populations ρ_{mm} (diagonal) and for the coherences $\rho_{m \neq m'}$ (off-diagonal).

Populations: The populations of the energy levels evolve according to:

$$\langle m | \dot{\rho}(t) | m \rangle = \sum_{k \neq m} (\Gamma_{mk} \langle k | \hat{\rho}(t) | k \rangle - \Gamma_{km} \langle m | \hat{\rho}(t) | m \rangle), \quad (10)$$

where Γ_{mk} represents the transition rate from state $|k\rangle$ to state $|m\rangle$ and is induced by the environment (reservoirs). This expression handles transitions in whichever basis one chooses and represents the net balance of population flows: gain from other levels minus loss to them.

Coherences: The coherences, on the other hand, are coupled both to the coherent (unitary) part of the system and to the environment, and evolve according to:

$$\langle m | \dot{\rho}(t) | m' \rangle = -\frac{i}{\hbar} \langle m | [\hat{H}_S, \hat{\rho}(t)] | m' \rangle - \frac{1}{2} \left(\sum_{\alpha \neq m'} \Gamma_{\alpha m'} + \sum_{\alpha \neq m} \Gamma_{\alpha m} \right) \langle m | \hat{\rho}(t) | m' \rangle, \quad (m \neq m'). \quad (11)$$

Initially, in the eigenbasis, these terms vanish. Depending on the system and the reservoirs, however, it is possible that coherences between the eigenstates are sometimes induced.

Finally, we can reduce the problem to an algebraic one:

$$\frac{d\rho_{ij}}{dt} = \sum_{kl} \mathcal{M}_{ij,kl} \rho_{kl}(t), \quad (12)$$

Stationary regime: In the stationary regime, we impose $\dot{\rho}_{ij} = 0$ for all elements. This allows us to rewrite the problem as a homogeneous linear system:

$$\mathcal{M}\vec{\rho} = 0, \quad (13)$$

where $\vec{\rho}$ contains all the elements ρ_{ij} and \mathcal{M} is the supermatrix that induces the transitions. We solve under the condition $\text{tr}(\rho) = 1$ (probability normalization).

3.5 Transition rates: Fermi's golden rule

The rates $\Gamma_{m \leftarrow n}$ are calculated to second order in the coupling by means of the bath correlation functions. In practice, we say that this is equivalent to applying Fermi's golden rule: the transition rate is proportional to the square of the interaction matrix element and to the density of states of the environment (at the relevant frequency). For example, if

$$V = \sum_k g_k |m\rangle\langle n| b_k + \text{h.c.} \quad (14)$$

(the important thing here is that we have an interaction with a term that induces the transition $n \rightarrow m$ while creating an excitation k in the bath), then

$$\Gamma_{m \leftarrow n} \sim \frac{2\pi}{\hbar} |g_k|^2 \delta(E_m - E_n \pm \hbar\omega_k), \quad (15)$$

where the delta enforces energy conservation between the system energy difference $E_m - E_n$ and the $\hbar\omega_k$ of the environment mode (absorbing or emitting a quantum). In continuous baths, the delta is interpreted as the environment spectral density $J(\omega)$ evaluated at the frequency $\omega_{mn} = (E_n - E_m)/\hbar$.

For a thermal bath (bosonic or fermionic), thermal occupation factors also appear: for instance, in a fermionic reservoir with Fermi distribution $f(\epsilon)$, a transition that gains an electron from the environment ($n \rightarrow m$ increasing the system occupation) has rate $\Gamma^+ \propto f(\hbar\omega_{mn})$, while the inverse one loses an electron with rate $\Gamma^- \propto 1 - f(\hbar\omega_{mn})$.

3.6 Current and entropy flows

Once the master equation is obtained, we can define flux observables between the system and its environments, which is what mainly interests us. In a quantum transport system, for example, we look for the charge or particle current that flows through the system, as well as the energy and heat flows towards the reservoirs, and the associated entropy production. From the Lindblad master equation, these quantities are computed using the transition rates:

Electronic current (I): If N_α is the particle number operator of reservoir α , the current flowing from α to the system (taken as positive in that direction) is defined as

$$I_\alpha = -e \frac{d}{dt} \langle N_\alpha \rangle = \frac{e}{\hbar} \text{Tr}([H_{\text{tot}}, N_\alpha] \rho_{SR}), \quad (16)$$

with the minus sign because a decrease in N_α implies current entering our system. Using the master equation and projecting onto the system's state basis, we obtain an expression in terms of the transition rates:

$$I_\alpha = e \sum_{m,n} (\Gamma_{m \leftarrow n}^{(\alpha)} P_n - \Gamma_{n \leftarrow m}^{(\alpha)} P_m), \quad (17)$$

where $P_n = \langle n | \rho_S | n \rangle$ is the population of the system state $|n\rangle$. Here $\Gamma_{m \leftarrow n}^{(\alpha)}$ is the rate at which the system transitions from n to m due to reservoir α . The difference $\Gamma^+ P - \Gamma^- P$

(where Γ^+ and Γ^- indicate whether the transitions increase or decrease the number of electrons transferred from the reservoir to the quantum system, respectively) reflects the net balance of particles entering minus those leaving. In the stationary state ($\dot{\rho}_S = 0$), this current is constant and equal to the one leaving through the other contacts (by charge conservation). For example, for a single quantum dot between two leads L and R in the stationary regime we have $I_L = -I_R$ (what enters through L exits through R). We thus find that charge is always conserved.

Energy flow (J^E): Analogously, we can define the energy flow from reservoir α to the system as $J_\alpha^E = -\frac{d}{dt}\langle H_\alpha \rangle$, where H_α is the Hamiltonian of environment α . Using the commutation with the total Hamiltonian, we arrive at a similar expression:

$$J_\alpha^E = \sum_{m,n} (\Delta E_{mn}) (\Gamma_{m \leftarrow n}^{(\alpha)} P_n - \Gamma_{n \leftarrow m}^{(\alpha)} P_m) . \quad (18)$$

Here $\Delta E_{mn} = E_m - E_n$ is the change in system energy in the transition $n \rightarrow m$, which corresponds to the energy extracted from the reservoir if $\Delta E_{mn} > 0$ (or given to the reservoir if $\Delta E_{mn} < 0$). This term weights the same rates as the particle current but multiplied by the energy transferred in each process.

Heat flow (J^Q): In thermodynamics, heat is the exchanged energy discounting the part associated with work. If reservoir α has a certain chemical potential μ_α , then exchanging particles also entails an energy exchange associated with electrical work $\mu_\alpha dN_\alpha$. For this reason we define the heat flow from α as energy minus work:

$$J_\alpha^Q = J_\alpha^E - \mu_\alpha I_\alpha . \quad (19)$$

This J_α^Q represents the rate of heat absorbed by the system from bath α (positive if the system gains energy not associated with work from the bath). In a single thermal bath, a positive J^Q indicates heat entering the system.

Work per reservoir: This is defined as the part of the exchanged energy that can be associated with ordered particle transport. The power for each reservoir α is:

$$\dot{W}_\alpha = \mu_\alpha I_\alpha , \quad (20)$$

where I_α is the particle current from reservoir α and μ_α its chemical potential. The term $\dot{W}_\alpha = \mu_\alpha I_\alpha$ represents the reversible work supplied by the environment. This useful energy, distinct from dissipated heat, allows us to analyze precisely the system's energy balance and the functional role of Maxwell's demons. This expression does not apply to phonon reservoirs, since they do not exchange conserved particles with the system. As they do not have a well-defined chemical potential, no form of reversible work can be associated with them.

Entropy flow and second law: A thermal reservoir at temperature T_α from which a heat dQ_α is extracted experiences an entropy change

$$dS_\alpha = -\frac{dQ_\alpha}{T_\alpha} \quad (21)$$

(negative if it gives off heat) according to Clausius' statement. Therefore, we define the entropy flow rate from the system to environment α as

$$\dot{S}_\alpha^{\text{fluo}} = -\frac{J_\alpha^Q}{T_\alpha}. \quad (22)$$

The total entropy production in the process (universe) is given by the sum of that produced in the system plus that in the environments. Using

$$\dot{S}_{\text{tot}} = \frac{d}{dt}(-\text{tr}(\rho_S \ln \rho_S)) + \sum_{\alpha} \dot{S}_\alpha^{\text{fluo}}, \quad (23)$$

one can show that for Lindblad-type dynamics $\dot{S}_{\text{tot}} \geq 0$, consistent with the second law of thermodynamics and where it seems that demons would not work, at least at the global scale. In the Markovian weak-coupling regime,

$$\dot{S}_{\text{tot}} = \dot{S}_S - \sum_{\alpha} \frac{J_\alpha^Q}{T_\alpha} \geq 0, \quad (24)$$

which corresponds to the standard irreversible description of the thermodynamics of quantum processes. In the stationary state ($\dot{S}_S = 0$), this expression implies

$$\sum_{\alpha} \frac{J_\alpha^Q}{T_\alpha} \leq 0, \quad (25)$$

that is, the heat flow satisfies the thermal equilibrium relation between multiple baths (a generalization of the Clausius criterion).

4 Autonomous system: conducting DQD with DQD trapdoor (quantum Smoluchowski)

This is the main system studied in this work, which, as mentioned later, can be considered an extension of Whitney's model in the referenced paper. We proceed to explain its Hamiltonian and its physical design, as well as its expected behavior.

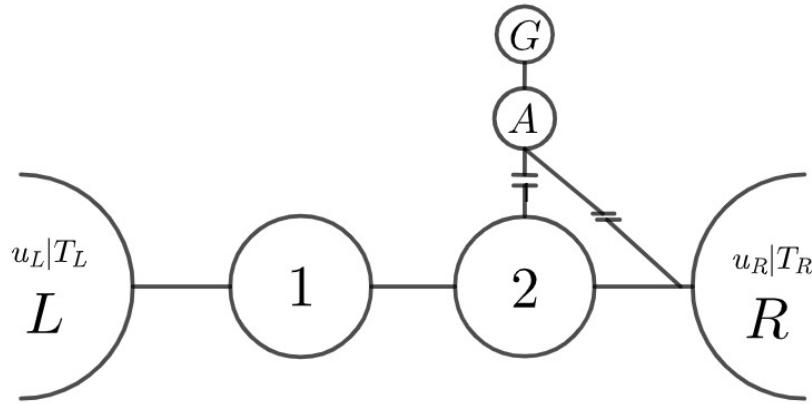


Figure 7: Scheme of the quantum system with electronic reservoirs L and R coupled, each with its own chemical potential and temperature. The conducting dots, called 1 and 2, are coupled and generate coherences between them, also allowing tunneling. In AG, the trapdoor DQD, they are separated from the conducting DQD, as they are only capacitively coupled. This implies that the electron in AG will never escape. A has a coupling with 2 and with the lead of reservoir R, to introduce Coulomb repulsion in 2 and at the entrance with R, “opening” or “closing” the door and availability of R.

In the following sections we will explain its physical operation and how it works as a demon.

4.1 Hamiltonian of the system

The system consists of a conducting double quantum dot and a lateral double quantum dot (A and G), coupled to each other and to two contacts (L and R). The total Hamiltonian has the following form:

$$\begin{aligned}
H = & \sum_{i=1,2} E_i D_i^\dagger D_i + E_A D_A^\dagger D_A + E_G D_G^\dagger D_G \\
& + \Gamma_{12}(D_1^\dagger D_2 + \text{h.c.}) + \Gamma_{AG}(D_A^\dagger D_G + \text{h.c.}) \\
& + E_C D_A^\dagger D_A D_2^\dagger D_2 + E_K D_1^\dagger D_1 D_2^\dagger D_2 + E_Z D_A^\dagger D_A D_G^\dagger D_G \\
& + \sum_{k,\alpha=L,R} \epsilon_{k\alpha} C_{k\alpha}^\dagger C_{k\alpha} \\
& + \sum_k (V_{kL} C_{kL}^\dagger D_1 + \text{h.c.}) \\
& + \sum_k (V_{kR} (1 - D_A^\dagger D_A) C_{kR}^\dagger D_2 + \text{h.c.})
\end{aligned} \tag{26}$$

Term by term:

- **Local energy:** $E_i D_i^\dagger D_i$ represents the energy associated with the occupation of dot i , and this is generalized for 1, 2, A, and G.
- **Coherent tunneling:**
 - Γ_{12} couples dots 1 and 2.
 - Γ_{AG} couples dots A and G.
- **Coulomb interactions:**
 - E_C penalizes the double occupation of A and 2 simultaneously. This term shifts the energies depending on whether dot 2 is occupied or not.
 - E_K penalizes the double occupation of 1 and 2.
 - E_Z penalizes the double occupation of A and G.
- **Contacts:** $\sum_k \epsilon_{kL} C_{kL}^\dagger C_{kL} + \sum_k \epsilon_{kR} C_{kR}^\dagger C_{kR}$ represents the energy of the electrons in the left (L) and right (R) contacts.
- **Coupling to contacts:**
 - V_{kL} allows exchange between the left contact and dot 1.
 - V_{kR} allows exchange between the right contact and dot 2, **only if dot A is empty** (factor $1 - D_A^\dagger D_A$).

This last term performs the function of a Maxwell demon: dot A blocks or allows the current depending on its occupation, thus controlling charge transfer in the system. It therefore functions as a quantum analogue of the Smoluchowski trapdoor, opening and closing (statistically) when it is advantageous.

In this Hamiltonian, we assume that E_K is sufficiently large for the system to be in the Coulomb blockade regime, such that 1 and 2 are never occupied at the same time. In the case of E_Z , it does not really matter, since it will not be coupled to any reservoir; its tunneling rate to the conducting DQD is negligible and it will only be coupled to a phonon reservoir; there will always be one electron in the trapdoor DQD that we denote by AG .

4.2 Phonon bath

As we will see in the discussion of results, the system requires a phononic coupling to dot AG in order to function as a demon. This can also be modeled at the Hamiltonian level in a similar way to the following:

$$H = \sum_q \omega_q b_q^\dagger b_q, ph + \sum_q (g_q b_q, ph^\dagger + g_q^* b_q, ph) (d_+^\dagger d_- + d_-^\dagger d_+) \quad (27)$$

Here, b_q^\dagger and b_q are the creation and annihilation operators of phonons in mode q , while g_q represents the coupling amplitude to the phonon mode. On the other hand, d_+^\dagger (d_+) and d_-^\dagger (d_-) are the creation (annihilation) operators of a particle in the states $|+\rangle$ and $|-\rangle$, respectively. The first term represents the free energy of the phonon bath, while the second describes energy exchange between the system and the environment, inducing transitions between the states $|+\rangle$ and $|-\rangle$. It is very important to note why we define these operators. $|+\rangle$ corresponds to the highest-energy eigenstate of AG and $|-\rangle$ to the lowest. We could have defined them with operators d_a^\dagger and d_g^\dagger , but it is more convenient to work in the eigenbasis of the lateral DQD.

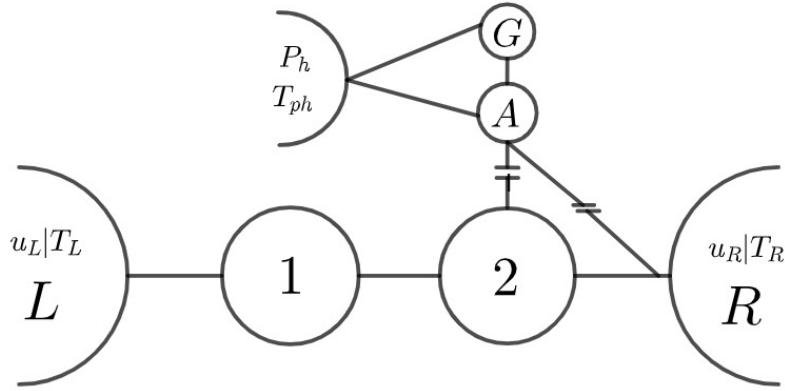


Figure 8: Extension of the system with a phonon reservoir coupled only to AG . This will couple the states as needed, moving the electron from the superposition of $+$ to $-$ and generating dynamics in the system, not simply leaving it in a “fixed” point. In reality, due to the superposition in the system, we are never completely in those states, but they serve as local bases in which to handle the ideas we seek in order to create the demon.

This coupling allows phonon emission and absorption processes that connect both eigenstates. The transitions between them have rates determined by the bosonic occupation distribution of the bath, according to:

$$\Gamma_{-\leftarrow+} = \gamma_{\text{ph}} [N_{\text{ph}}(|\Delta E|) + 1] \quad (28)$$

$$\Gamma_{+\leftarrow-} = \gamma_{\text{ph}} N_{\text{ph}}(|\Delta E|) \quad (29)$$

where $N_{\text{ph}}(\Delta E) = (e^{\beta \Delta E} - 1)^{-1}$ is the average phonon occupation with energy ΔE (with $\beta = 1/K_B T$), and γ_{ph} encapsulates the effective coupling to the bath. These rates reflect spontaneous and stimulated phonon emission and absorption that induce dissipative dynamics between the energy states of the system.

4.3 A “small” complication

In this system, an important complexity arises: the transitions induced by the coupling to the phonon bath not only modify the populations of the system eigenstates, but also induce coherences between the eigenstates themselves. This is because the system has 6 eigenstates, 4 corresponding to the conducting DQD filled and 2 corresponding to it empty, of which the first 4 are superpositions of all local states $|1A\rangle$, $|1G\rangle$, $|2A\rangle$, and $|2G\rangle$. Consequently, it is not possible to treat the phononic transitions in a purely population-based way; a description including quantum coherences is required.

To address this small inconvenience, it is necessary to model the system dynamics using a Lindblad-type superoperator formalism, as discussed earlier, acting on the full density matrix ρ in the eigenbasis. This approach allows one to properly capture the dissipative and coherence effects induced by this phonon bath.

The procedure followed is as follows:

1. First, the full Hamiltonian of the system is diagonalized in the local basis $\{|1A\rangle, |1G\rangle, |2A\rangle, |2G\rangle, |0A\rangle, |0G\rangle\}$, thus obtaining the eigenstates and eigenenergies that define the final basis of the system.
2. To describe the coupling to phonons, it is useful to define an intermediate *mixed* basis in the AG subsystem, for each occupation configuration of the conductor (1, 2). Given a mixing angle θ_i , where $\theta_1 = \theta_0 = \arctan\left(\frac{2|\Gamma_{AG}|^2}{E_A - E_G}\right)$ and $\theta_2 = \arctan\left(\frac{2|\Gamma_{AG}|^2}{E_A + E_C - E_G}\right)$, the energy eigenstates of the AG subsystem are defined as:

$$|+\rangle_i = \cos(\theta_i/2)|A\rangle + \sin(\theta_i/2)|G\rangle \quad (30)$$

$$|-\rangle_i = -\sin(\theta_i/2)|A\rangle + \cos(\theta_i/2)|G\rangle \quad (31)$$

The inverse of this transformation is:

$$|A\rangle = \cos(\theta_i/2)|+\rangle_i - \sin(\theta_i/2)|-\rangle_i \quad (32)$$

$$|G\rangle = \sin(\theta_i/2)|+\rangle_i + \cos(\theta_i/2)|-\rangle_i \quad (33)$$

This formulation is applied separately to the configurations with 1 in dot 1, in dot 2, and in neither, generating angles θ_1 , θ_2 , and θ_0 , respectively.

3. The change-of-basis matrix T is then constructed from the local basis to the mixed basis $(1+, 1-, 2+, 2-, 0+, 0-)$, in block form. Each block is a 2×2 rotation matrix

with the corresponding angle:

$$T = \begin{pmatrix} \cos(\theta_1/2) & -\sin(\theta_1/2) & 0 & 0 & 0 & 0 \\ \sin(\theta_1/2) & \cos(\theta_1/2) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos(\theta_2/2) & -\sin(\theta_2/2) & 0 & 0 \\ 0 & 0 & \sin(\theta_2/2) & \cos(\theta_2/2) & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos(\theta_0/2) & -\sin(\theta_0/2) \\ 0 & 0 & 0 & 0 & \sin(\theta_0/2) & \cos(\theta_0/2) \end{pmatrix} \quad (34)$$

4. The phononic operator in the mixed basis is defined as an operator that induces transitions between the states $|+\rangle$ and $|-\rangle$ of each subspace, represented in matrix form as:

$$O_{\text{fonon, mixta}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (35)$$

It is defined through the jump operators:

$$\sum_{i=0}^2 (|i+\rangle\langle i-| + |i-\rangle\langle i+|) \quad (36)$$

This operator induces coherent transitions between the eigenstates of the AG subsystem for each configuration of the conductor occupation (1, 2), labelled by the index i . In this way, the phonon bath is coupled only to the lateral subsystem AG and does not directly affect the conducting DQD. This choice allows a clear separation between the thermodynamic mechanism of the demon (based on AG) and the main conducting system, avoiding interference between both processes.

5. Now, this operator is transformed to the system eigenbasis via:

$$O_{\text{ph}} = V^\dagger T^\dagger O_{\text{fonon, mixta}} T V \quad (37)$$

where V is the matrix whose column vectors are the eigenstates obtained by diagonalizing the total Hamiltonian. .

6. With this transformed operator, the transition rate matrix between eigenstates, W_{ij} , is defined using the formula:

$$W_{ij} = \phi |\langle i | O_{\text{ph}} | j \rangle|^2 N_{\text{ph}}(\Delta E) \quad (38)$$

depending on whether it is an absorption ($\Delta E > 0$) or emission ($\Delta E < 0$) process, with $N_{\text{ph}}(\Delta E)$ the corresponding bosonic distribution.

7. Finally, from W_{ij} , the Lindblad jump operators L_{ij} are constructed:

$$L_{ij} = \sqrt{W_{ji}} |i\rangle\langle j| \quad (39)$$

and with them the dissipative superoperator \mathcal{D} is defined as:

$$\mathcal{D}(\rho) = \sum_{i \neq j} \left(L_{ij}\rho L_{ij}^\dagger - \frac{1}{2}\{L_{ij}^\dagger L_{ij}, \rho\} \right) \quad (40)$$

This supermatrix \mathcal{D} is discretized as a $6^2 \times 6^2$ matrix, acting on the vectorized space of the density matrix.

This treatment allows an accurate description of the system's dissipative dynamics, including both the transition rates and the coherence effects induced by the phonon bath. The resulting stationary equation is:

$$(M + \mathcal{D})\rho = 0 \quad (41)$$

with M the superoperator associated with the coupling to the electronic contacts and \mathcal{D} that of the phononic coupling, as just described.

It is important to mention that the Lindblad equation is in the secular approximation, so M does not add coherences due to the phonon bath. It will be a 6×6 that we will extend with zeros computationally.

4.4 Why this model?

This model is inspired by Whitney's quantum Smoluchowski trapdoor proposed in his work. The main goal is to regulate the electronic flow through contact 2 with reservoir R , acting analogously to an intelligent trapdoor.

To this end, the capacitive interaction term E_C is introduced, which allows us to modify the energies of the lateral subsystem AG depending on the occupation of dot 2. When this dot is occupied, the energy of level A is shifted by E_C , which can better align the conditions for the electron to leave the system towards reservoir R (adjusting its proximity to the chemical potential μ_R). In contrast, when dot 2 is empty, this shift disappears, moving the relevant energies away from the transport window and making it more difficult for an electron to exit through that channel.

Furthermore, the factor $1 - D_A^\dagger D_A$ appearing in the coupling Hamiltonian between dot 2 and reservoir R acts as a tunneling modulation factor, cancelling the coupling when level A is occupied. This mechanism reinforces the effective disconnection between the conductor and the environment when the demon is “active”, i.e., when it stores an electron in dot A .

Taken together, these two ingredients allow the demon's operation (flow control in AG) to be separated from the main transport channel (dots 1 and 2), thus playing a key role in the thermodynamics of the system.

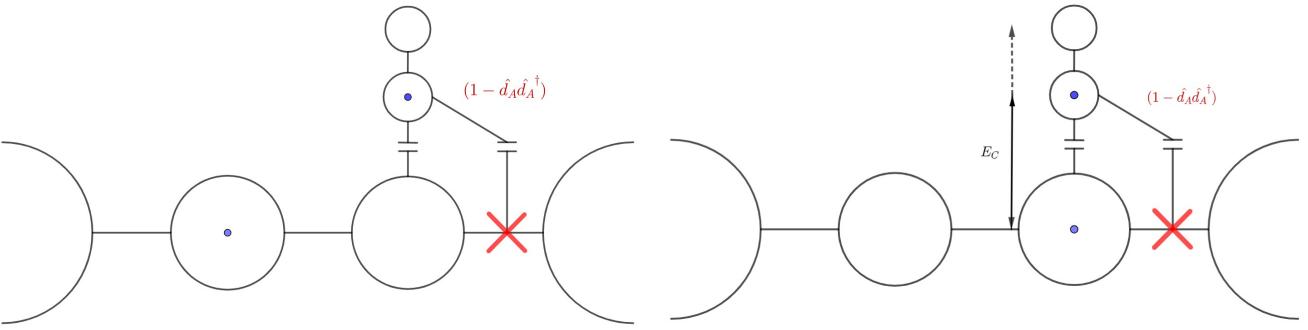


Figure 9: Effect of the electron in A on the system. If it is in A, the operator forbids the transition of electron entry or exit. When the conducting electron moves to 2, there is an additional Coulomb repulsion energy E_C in the system, which will shift A and open the door to R.

Sequentially, the system can be understood as:

1. The electron in the lateral system is mostly localized in dot A.
2. A new electron enters through dot 1, since entry through 2 is much less probable due to the energetic design of the system.
3. The electron in 1 tunnels to dot 2.
4. Upon reaching dot 2, the strong repulsion with the electron in A induces a transition of the electron from A to G.
5. This change activates the capacitive coupling, readjusting the energy of the level in 2.
6. As a consequence, the coupling door to reservoir R opens, facilitating the exit of the electron from 2 to that reservoir (although there is also the possibility for the electron to return to 1).

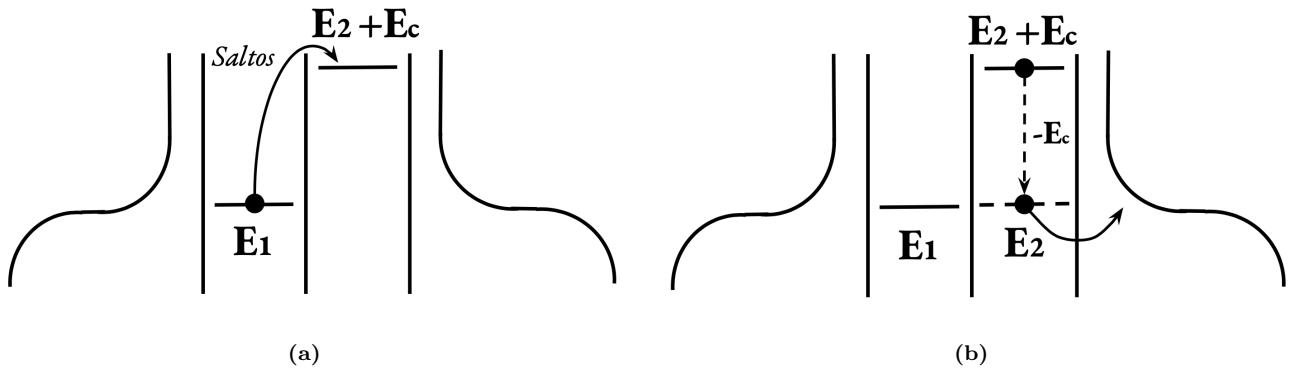


Figure 10: Resonance scheme. In figures (a) and (b) it can be seen that the jump of the electron from dot 1 to 2 implies an energy cost due to Coulomb interaction with an electron in dot A. Once the system statistically reaches state 2 and the trapdoor electron moves to G, the conducting electron can exit to R with higher probability, “opening” the door. This analysis has been performed by fixing $E_1 = E_2$, although other cases will also be studied to understand their influence.

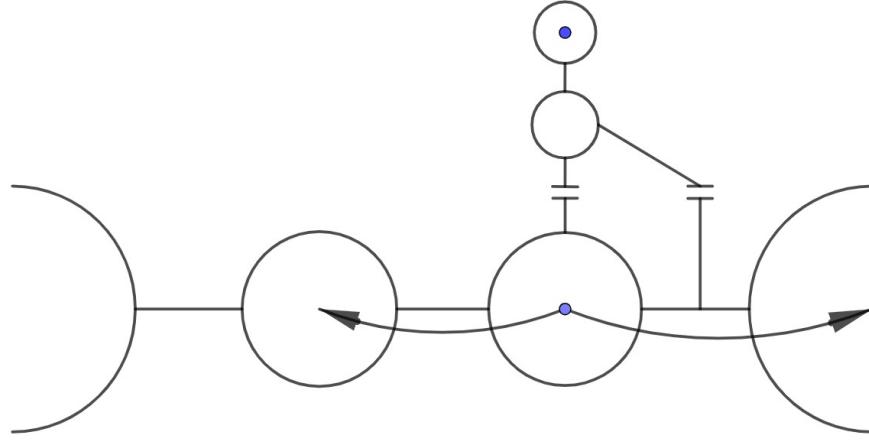


Figure 11: The system opens!

This is key, since Whitney found that, although his demon worked well in terms of moving the particle flow, there was an energy exchange between meter and demon, so it was not a pure demon and worked as a heat engine. Now then, can the fact of incorporating a conducting DQD instead of Whitney's simple QD make the system function not only as a thermal machine?

This is the main motivation for studying this system. In fact, we will realize that there are several different scenarios for resonance that may be interesting in the system depending on what is sought. In the following figures, the other main case of interest is shown:

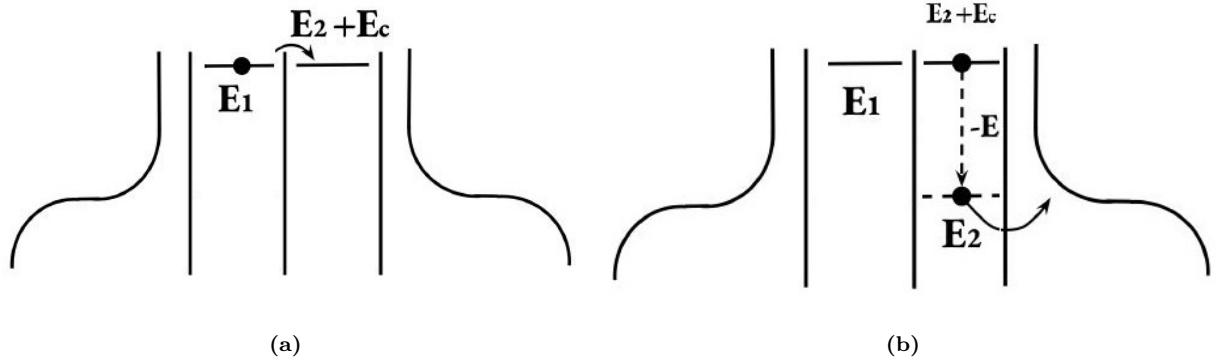


Figure 12: Scheme of the other resonance. The idea is the same, but the difference is that the jump between conducting dots is more favorable and does not require that extra energy. In both cases, the chemical potentials have to be tuned to favor or suppress the system transitions with the reservoirs.

5 Results and discussion

Before starting, it is important to verify that the demon is capable of generating a net current even under isothermal conditions ($T_L = T_R$) and with equal chemical potentials ($\mu_L = \mu_R$). It is precisely in this configuration that one can guarantee that the system exhibits an effective asymmetry induced solely by the demon.

5.1 Basic operation and phonon bath

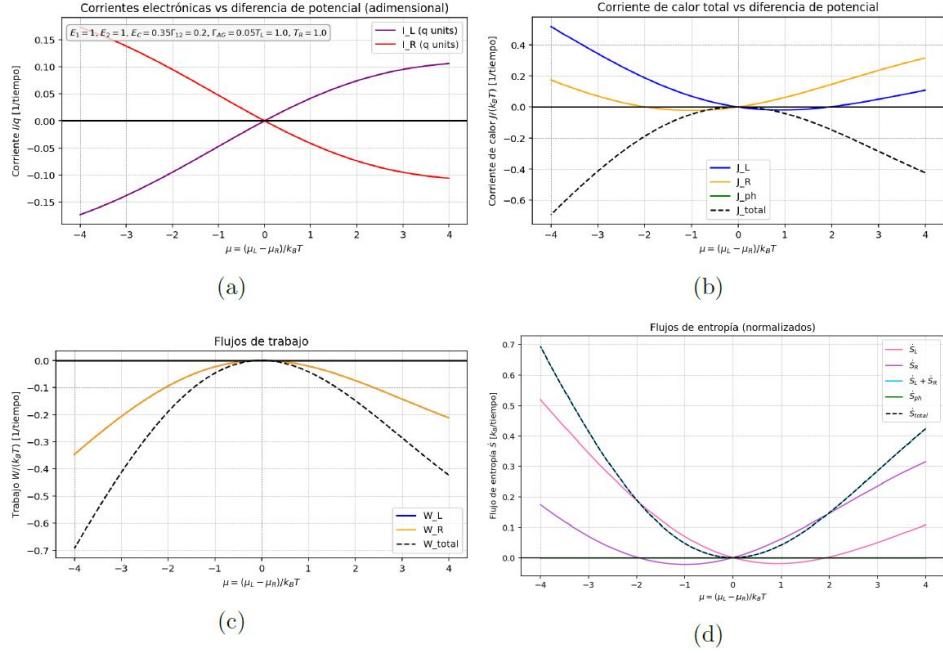


Figure 13: Representation of the different thermodynamic variables for the system without phonon bath. The plots are normalized to an undefined natural time unit and in units of $k_B T$ or k_B , which are set to 1.

Looking at the system without coupling to the phonon bath, we see that at $\mu = 0$ there is no current flow; therefore, equilibrium is reached and the demon does not work. There is no sustained net current that would be produced by a demon. This can be seen in the plots of the work or heat currents, where the dashed line represents the power exerted on the system, which has a maximum of 0 at $\mu = 0$. Consequently, the entropy is not reduced even in the conducting DQD (locally) and the total entropy respects the second law.

In essence, we have just replicated the Smoluchowski trapdoor in a quantum system and see its expected effects: the conducting DQD does not generate asymmetries. This is why we need the phonon bath to couple the “oscillations” of the trapdoor and generate these asymmetries.

A very important phenomenon to keep in mind is the presence of regions where the entropy of each reservoir can decrease below 0, even though in total it is greater than zero. This is simply a consequence of the heat flow in the system. In the end, we are modulating the chemical potentials for this effect.

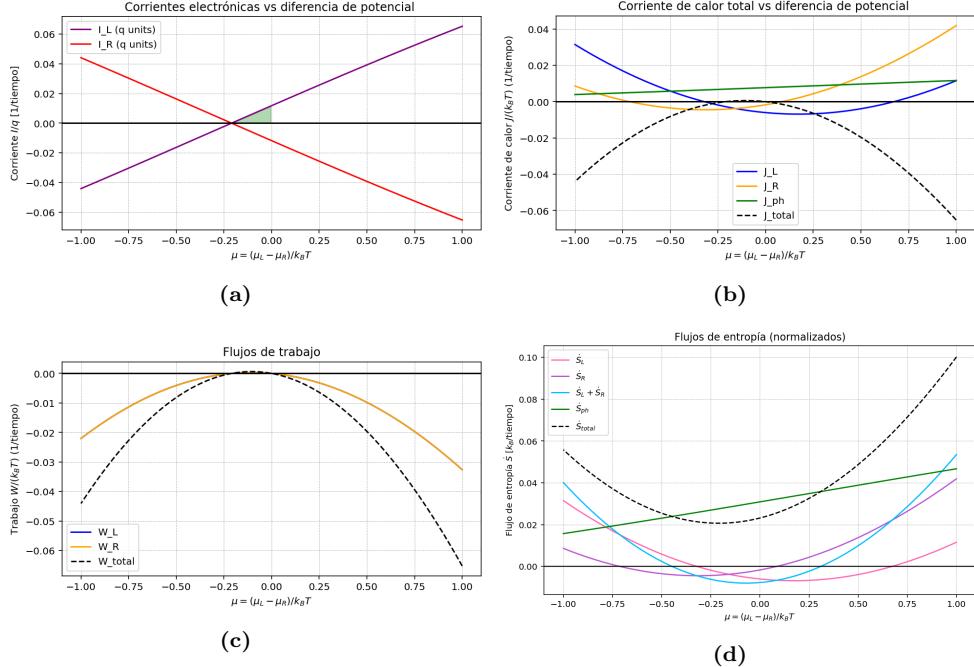


Figure 14: Same system but now with a phonon reservoir inducing 36×36 transitions. The relevant parameters have been exaggerated to better see the demon’s effects. The reservoir temperature is multiplied by 4, and the phonon temperature is 40 times lower. The energies of the conducting dots are multiplied by 1.2.

Before discussing the results, it is important to mention that, in the computation of the phonon-bath superoperator matrix, there are very few coherent terms between eigenstates of the system in the 36×36 matrix, with the terms being mainly diagonal. We are therefore working in the secular regime.

As can now be seen in plot (a), there is a region of imbalance where the current is greater (or smaller) than it would be without the demon’s effect. Asymmetry has been achieved! We have coupled the trapdoor and now the system has a preferred flow; the demon is working.

The physical mechanism can be understood via the Smoluchowski trapdoor. If we were to couple our original trapdoor to a cold medium, it would be less affected by random motion and would let particles pass selectively. In our case, we cool our trapdoor QD and obtain the same effect, redirecting the flow.

Even so, from the heat current of the bath we can see that, indeed, it behaves more like a thermal machine than a simple “selector”. One can see the region in which the system performs positive power and, in general, the phonon bath exchanges energy with the system in the form of heat. This power is used to go against the chemical potential gradient and is denoted by the green region in figure 14 (a).

Although the main goal in this situation could be to minimize the heat exchange with the phonon bath, it is interesting to analyze the local entropy flows, \dot{S}_L and \dot{S}_R . In plot (d), it is observed that the sum $\dot{S}_L + \dot{S}_R$ can reach negative values even outside the domain where net work is performed ($W_{total} > 0$). This indicates that, locally, the system can act as an effective demon: it reduces entropy in the electronic contacts without necessarily producing useful work. This expanded region of negative local entropy suggests that the asymmetry induced by the coupling to the bath allows some degree of local order, with the system functioning as a refrigerator without generating power.

In short, the system can display demonic behavior in a local sense, without violating

the global second law thanks to the dissipative role of the phonon bath. In other words, the entropy reduction in the reservoirs due to the trapdoor in this non-power regime is transferred as heat to the phonon bath, where it is dissipated.

5.2 Resonance analysis

From now on, $K_B T$ will be used as the energy reference. We now aim to study whether an autonomous demon that does not exchange heat with the phonon bath is possible in our system. To do so, we seek to minimize the function J_{ph} with respect to other variables and for different resonance conditions. We also analyze the physical meaning of a possible case in which $J_{ph} = 0$.

We will first analyze a case with a phonon bath temperature equal to the temperature of the two reservoirs and then return to the cold case.

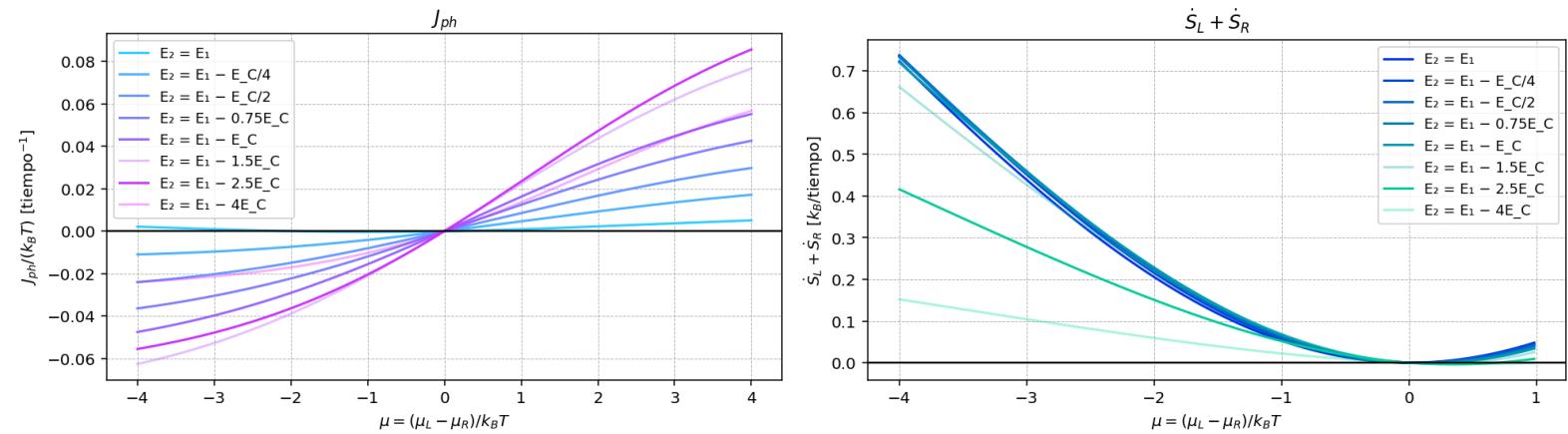


Figure 15: (a) Representation of the heat transmitted by the phonon bath at a temperature equal to that of the reservoirs for different resonance cases. (b) Same representation for the local entropy of the conducting DQD.

It can be seen that, for no resonance, the demon works at the local level in this case (the minimum local entropy is zero). It has been verified (see references) that only with a phonon reservoir with $T_{ph} < T$ can one obtain the demon effect. In any case, all minima in panel 15 (b) occur at $\mu = 0$ and are equal to 0.

The sign change in $\mu = 0$ for the phonon heat confirms that the system is indeed following a preferred direction and that the trapdoor is not selecting. We simply have a thermoelectric quantum system with a selected flow.

The difference between resonances, for now, only informs us about the amount of heat or entropy we want to have in our system, but since it is not yet a functional demon, this is not useful for this work.

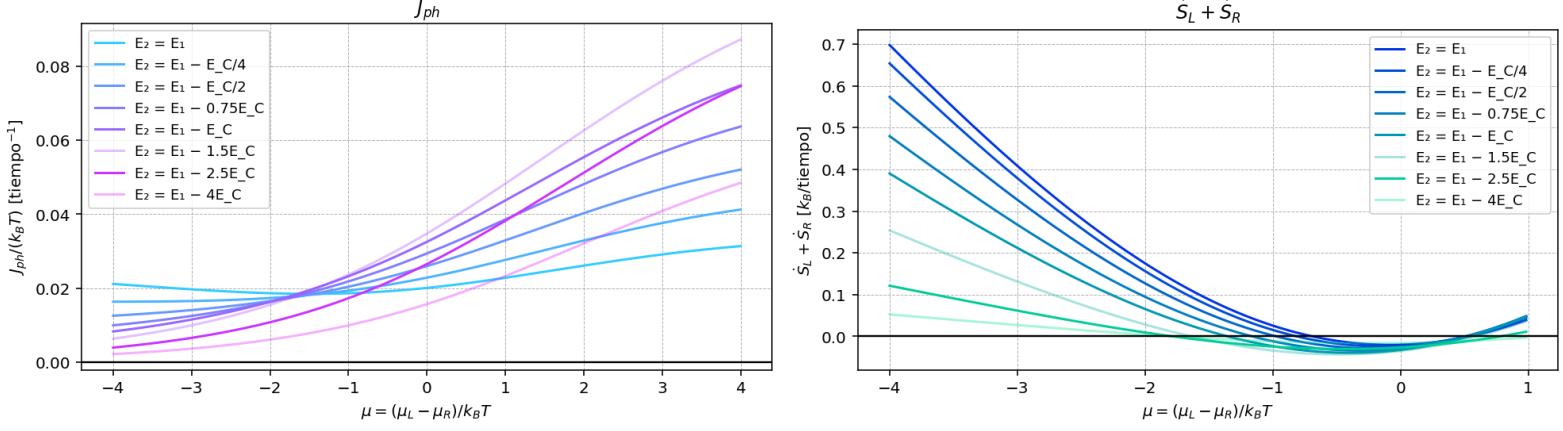


Figure 16: Representation of the previous figure for the same resonances with a cold phonon bath at $T_{ph} = 0.1T_{ref}$, the latter being the reservoir temperature.

Here the effects due to the cold phonon bath for all resonances begin to appear. There is an asymmetry in the heat current at $\mu = 0$, as can be seen in figure 14.

The minima of local entropy oscillate between fairly similar values for this temperature value. Depending on the desired range of μ , it is convenient to use one or another resonance. In any case, it does not seem possible to achieve a perfect resonance in which the demon operates without exchanging heat.

From now on, we will mainly analyze the resonances mentioned in the theoretical introduction: $E_1 = E_2$ and $E_1 = E_2 - E_C$. This choice is made because the minimum entropy of all resonances seems to be bounded by $E_1 = E_2 - 1.5E_C$, but the difference is very small ($\Delta S_{\min} \approx 3.63 \times 10^{-3}$). In the other case, we use $E_1 = E_2$ because its entropy minimum is at $\mu = 0$, with the rest being shifted to the left and below this and acting as an upper bound for the other minima in the resonance. In this way, all possible resonances (unless they are very extreme) will be located between these two.

Resonance	$ J_{ph}/(\dot{S}_L + \dot{S}_R) _{\min}$
$E_2 = E_1$	0.9786
$E_2 = E_1 - \frac{E_C}{4}$	0.9247
$E_2 = E_1 - \frac{E_C}{2}$	0.8552
$E_2 = E_1 - 0.75E_C$	0.7856
$E_2 = E_1 - E_C$	0.7274
$E_2 = E_1 - 1.5E_C$	0.6797
$E_2 = E_1 - 2.5E_C$	0.7366
$E_2 = E_1 - 4E_C$	0.8642

Table 1: Ratio $|J_{ph}/(\dot{S}_L + \dot{S}_R)|$ at the point of minimum total electronic entropy for different resonances in Figure 19.

It is important to mention that these results suggest a physical minimum of entropy as a function of the resonance, with a preferred resonance. It is believed that this will simply depend on the Hamiltonian parameters and differences between the eigenenergy levels of the Hamiltonian.

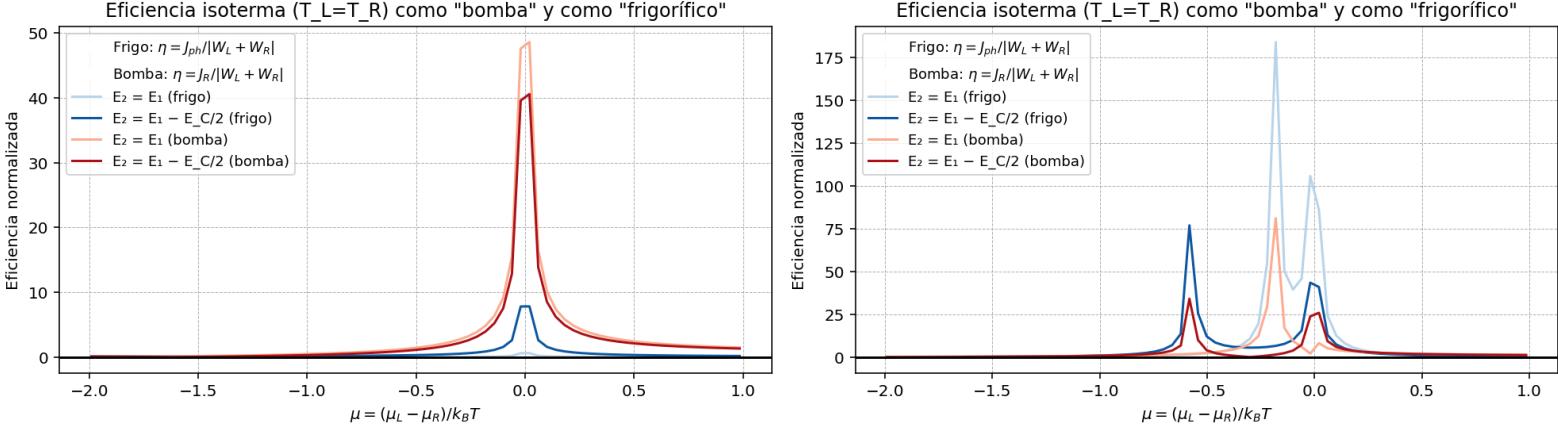


Figure 17: Analogues of thermal efficiency for the two main resonances for a reservoir at $T_{ph} = T_{ref}$ (a) and a cold reservoir (b).

They are not actual definitions of efficiency as such, because the cold bath is not being cooled in a refrigerator nor the hot one heated in a heat pump; they are useful analogues for the study. If we now analyze different forms of efficiency for the system, since even in the isothermal case we can analyze the ratios shown in the figure, we again find several differences between the hot and cold cases. The hot case has been represented in order to see the formation or displacement of peaks for the cold bath and to see that, as might be expected, the system with the cold bath works better as a refrigerator and not so much as a pump.

Looking at plot 17 (b), in general there seems to be a higher ratio of heat absorbed by the bath for the resonance $E_1 = E_2$. This can be useful if we accept the demon's role as a thermal machine, but not if we continue to seek to minimize the exchanged heat while maintaining the local entropy reduction.

Thus, given all the information in this section, it does not seem possible to completely eliminate the exchanged heat, although several efforts can be made to minimize this quantity.

5.3 Region analysis

Up to now, we have analyzed power regions, demon-action regions, minimization of J_{ph} ... The existence of a demon under certain conditions has been found. We now propose to perform a more exhaustive analysis of the system, varying the values of μ as before in the reservoir temperature space up to $T_{ph} = 2T_{ref}$. In this way, for the different resonances, we can look for power regions, local negative entropy regions, lines of vanishing energetic quantities, and look for relationships between these.

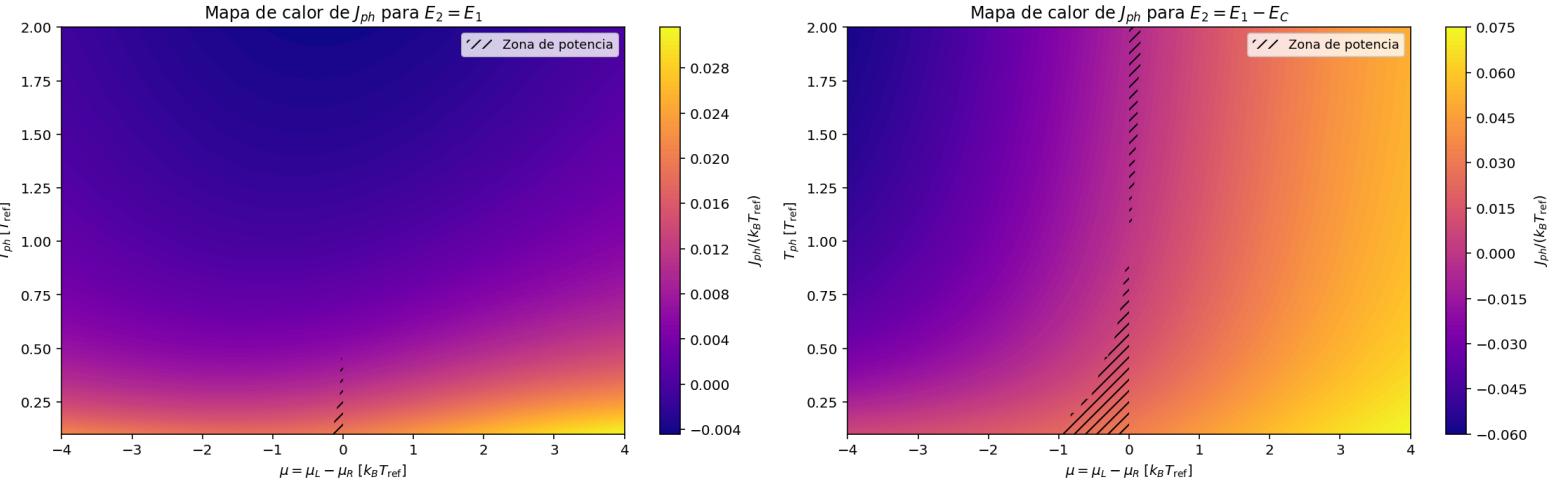


Figure 18: Normalized maps for J_{ph} for the two main resonances considered. The region of positive power is shown for $P > 0$.

The first thing to highlight from these plots is that we can minimize the heat J_{ph} for the first resonance. As we have already seen and will continue to see, the entropy maps take very similar values over all T_{ph} and μ , so it may be useful to work in resonances close to $E_1 = E_2$. In any case, and continuing the analysis, the power regions are much smaller for these resonances, which can be a disadvantage. As we saw earlier, we do not necessarily have to be in these regions for the demon to work, but in a complicated experimental setup, it would be better to have a larger margin of maneuver.

Another interesting result is the formation of power regions with positive μ in $T_{ph} > T_{ref}$, but these never connect for any value of T_{ph} in any resonance and do not reduce entropy locally (this will be seen in plot 22).

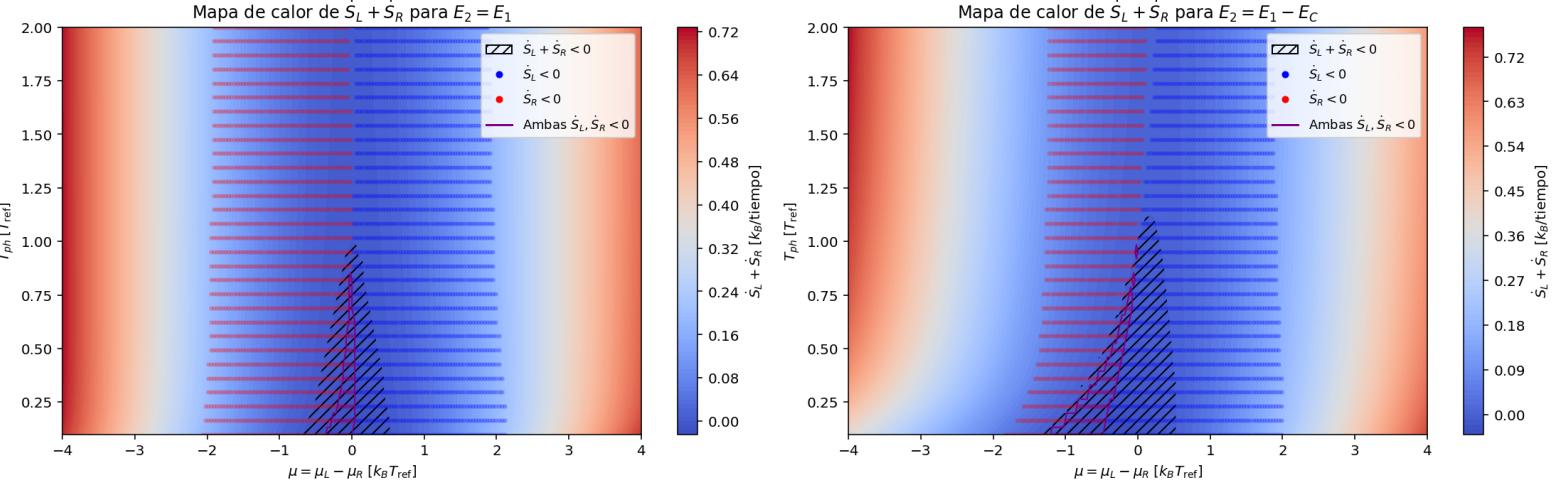


Figure 19: Normalized entropy maps for the two configurations.

There is very relevant information in these two plots. To begin with, the bath temperature generally has to be lower than the reference temperature, but there is a demon region in $T_{ph} > T_{ref}$ for the second resonance! This result can be very useful in the setup of these systems, since cooling reservoirs so much can be very difficult. Furthermore, it is a purely quantum result; this could not happen in the original Smoluchowski trapdoor.

On the other hand, there are regions where both are negative, so our system could be operating on both reservoirs, which would also be impossible in the original trapdoor. This effect is very reminiscent of the first pressure and temperature demons. In reality, the phonon bath is compensating with even more heat and entropy, respecting the second law, but it remains very useful to know that there are regions where we can reduce the entropy of both conducting reservoirs.

E_2	% región ocupada	μ (región $\dot{S}_L + \dot{S}_R < 0$)		T_{ph} (región $\dot{S}_L + \dot{S}_R < 0$)		μ (región $\dot{S}_L, \dot{S}_R < 0$)		T_{ph} (región $\dot{S}_L, \dot{S}_R < 0$)	
		min	max	min	max	min	max	min	max
E_1	19.83 %	-0.66	0.50	0.10	0.95	-0.34	0.02	0.10	0.82
$E_1 - \frac{1}{4}E_C$	21.12 %	-0.78	0.50	0.10	0.95	-0.54	-0.02	0.10	0.89
$E_1 - \frac{1}{2}E_C$	20.50 %	-0.94	0.50	0.10	1.02	-0.74	-0.02	0.10	0.89
$E_1 - \frac{3}{4}E_C$	21.90 %	-1.15	0.50	0.10	1.02	-0.98	-0.02	0.10	0.89
$E_1 - E_C$	22.32 %	-1.35	0.50	0.10	1.08	-1.19	-0.02	0.10	0.95
$E_1 - 1.5E_C$	27.33 %	-1.63	0.58	0.10	1.21	-1.51	-0.02	0.10	0.95
$E_1 - 2.5E_C$	42.31 %	-1.75	0.74	0.10	1.34	-1.71	0.02	0.10	0.95
$E_1 - 4E_C$	76.26 %	-1.75	1.11	0.10	1.41	-1.75	0.94	0.10	1.21

Table 2: Negative entropy regions.

This table extends the information in plot 22 for all resonances in order to analyze the ranges in which they exist and their relationship with the “double demon” region ($\dot{S}_L, \dot{S}_R < 0$). The occupied region is the percentage of demon region (negative entropy) that it covers. For demons with lower resonances, the occupied region tends to increase compared to the total. Additionally, for these, the temperature and μ ranges where these total and partial regions exist also increase.

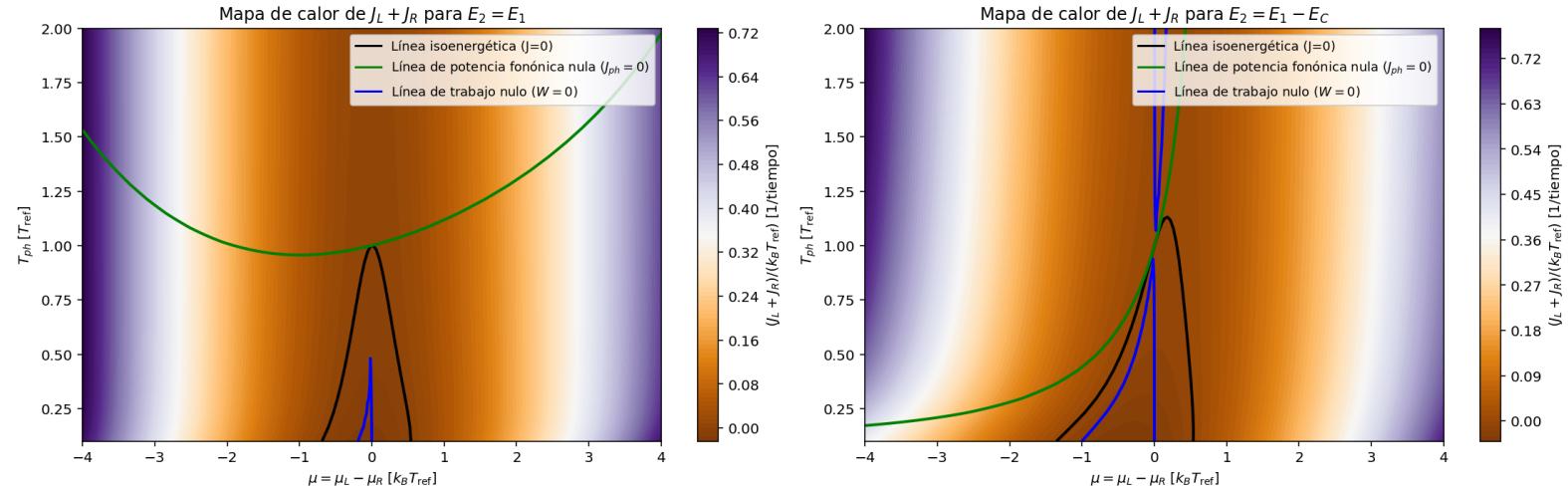


Figure 20: Map of $J_L + J_R$ for the two resonances. The isoenergetic line is the line where $J_L + J_R = 0$. It is called so for convenience.

Finally, looking at the map of $J_L + J_R$, the isoenergetic line where this sum is zero has been shown, enclosing the demon area (negative local entropy) together with the zero-work region in the system and the line of zero phononic heat.

Before going on, it is necessary to mention that the program diverges numerically for the work function around $\mu = 0$. In that region the work should follow the line of the other two. It is recommended to consult the plots in the appendices for other resonances

to see how this divergence decreases in other cases. Thus, the region between the triple points is interpreted as a line (or a point for the first resonance) where they become equal, as this is what makes physical sense.

The region in which this happens coincides with the dynamic stability region of the system. The ideal demon could only exist if the green line crossed the black one below its maximum at some point, entering the area of negative local entropy. This does not happen for any resonance and confirms once and for all that this demon is a thermal demon, which operates via heat exchange. We can be near the equilibrium point of $\Delta\mu$ and T_{ph} to minimize the exchanged heat and, as we have seen, for low resonances, this region can be close to or coincide with that of the “double demon”, or at least with that of negative entropy, since around those regions the values remain considerably close to their (negative) minima.

5.4 A possible alternative

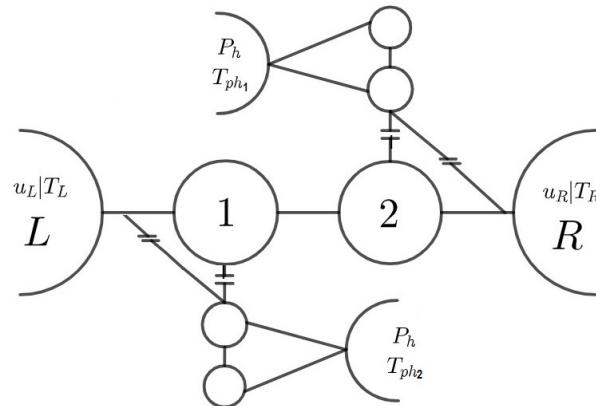


Figure 21: Possible scheme of an effective ideal demon.

Thanks to the study of this system, the existence of a demon with two trapdoors coupled to their respective phonon baths is proposed for future research. If the heat exchanged with one were the opposite of that with the other, there would be no net exchange with the conducting DQD, thus restoring the “ideal” demon.

6 Conclusions

The system acts as a functional quantum Smoluchowski trapdoor in which an asymmetric flow is allowed through the incorporation of a phonon bath (not necessarily cold) that regulates its randomness and in which new effects arise, considered impossible in the non-quantum trapdoor. The trapdoor exchanges energy in the form of heat with the conducting system indirectly.

The resonances used affect not only the shape but also the amount of heat exchanged with the phonon bath, which can be minimized, while the minimum local entropy flux values come much closer together, allowing one to choose whichever case is most convenient.

The demon can reduce the entropy of both electronic reservoirs, even near the isoenergetic line (depending on the resonance).

The isoenergetic line never passes through the local negative-entropy (demon) area, which makes an ideal (non-thermal) demon impossible, and allows the demon to be interpreted as a thermal machine that would use microscopic information about the system to operate. This is why a possible system with no net energy exchange is proposed.

References

- [1] R. Sánchez Rodrigo, *Spin and Charge Transport through Driven Quantum Dot Systems and their Fluctuations*, Doctoral Thesis, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 2007.
- [2] R. S. Whitney, *Illusory Cracks in the Second Law of Thermodynamics in Quantum Nanoelectronics*, Laboratoire de Physique et Modélisation des Milieux Condensés, Université Grenoble Alpes and CNRS, April 2023.
- [3] L. H. Willems van Beveren, *Electron spins in few-electron lateral quantum dots*, Doctoral Thesis, 2005.
- [4] J. Darulová, *Automated Tuning of Gate-defined Quantum Dots*, Doctoral Thesis, ETH Zurich, 2020.
- [5] A. de Oliveira Junior, J. B. Brask, R. Chaves, *A friendly guide to exorcising Maxwell's demon*, Technical University of Denmark, Federal University of Rio Grande do Norte, March 2025.
- [6] P. S. Pal, A. M. Jayannavar, *Maxwell's Demon, Szilard Engine and Landauer Principle*, University of Maryland, Institute of Physics Bhubaneswar, Homi Bhabha National Institute, April 2019.
- [7] J. D. Norton, *Eaters of the lotus: Landauer's principle and the return of Maxwell's demon*, Department of History and Philosophy of Science, University of Pittsburgh, 2004.
- [8] R. El Skaf, *What notion of possibility should we use in assessing scientific thought experiments?*, *Lato Sensu: Revue De La Société De Philosophie Des Sciences*, Vol. 4, No. 1, July 2017.
- [9] R. Sánchez, P. Samuelsson, and P. P. Potts, *Autonomous conversion of information to work in quantum dots*, Phys. Rev. Research **1**, 033066 (2019).
- [10] J. Monsel, M. Acciai, R. Sánchez, and J. Splettstoesser, *Autonomous demon exploiting heat and information at the trajectory level*, Chalmers University of Technology, 2024.
- [11] W. G. van der Wiel et al., *Electron transport through double quantum dots*, Published 17 December 2002.
- [12] N. Freitas and M. Esposito, *Characterizing autonomous Maxwell demons*, March 17, 2021.
- [13] G. Benenti, G. Casati, K. Saito, and R. S. Whitney, *Fundamental aspects of steady-state conversion of heat to work at the nanoscale*.

- [14] T. Sagawa, *Thermodynamics of Information Processing in Small Systems*, Kyoto University, October 24, 2011.
- [15] G. Schaller, *Open Quantum Systems Far from Equilibrium*, Lecture Notes in Physics, Springer, ISBN 978-3-319-03876-6.
- [16] R. Sánchez and M. Büttiker, *Optimal energy quanta to current conversion*, Département de Physique Théorique, Université de Genève, August 17, 2018.
- [17] P. P. Potts, *Quantum Thermodynamics*, Department of Physics and Swiss Nanoscience Institute, University of Basel.
- [18] R. Sánchez, J. Splettstoesser, and R. S. Whitney, *Non-equilibrium System as a Demon*, December 9, 2019.
- [19] T. Fujisawa, T. Hayashi, and S. Sasaki, *Time-dependent single-electron transport through quantum dots*, Rep. Prog. Phys. **69**, 759 (2006).
- [20] C. W. J. Beenakker, *Theory of Coulomb-blockade oscillations in the conductance of a quantum dot*, Phys. Rev. B, 1991.

Appendix: Analysis of Feynman's Ratchet

The system consists of a toothed wheel (ratchet) connected to a common axis with a paddle immersed in a gas at temperature T_1 , while the ratchet is in contact with another gas at temperature T_2 . The wheel can rotate freely, but is blocked by the ratchet depending on the direction.

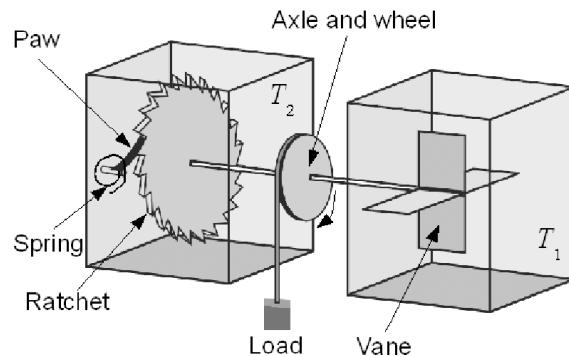


Figure 1: Scheme of the ratchet-pawl

1. Physical variables

- T_1, T_2 : temperatures of the gases surrounding the paddle and the ratchet, respectively.
- ω : angular rotation velocity of the axis.
- N : number of ratchet teeth.
- θ : rotation angle.
- τ : torque applied on the axis.
- E : energy required to compress the spring of the ratchet.
- r : radius of the axis, L : length of the paddle.

2. Transition rates

The forward jumping rate (favoured by T_1) is proportional to the thermal probability of overcoming the energy E :

$$R_+ = R_0 \exp\left(-\frac{E - \tau\theta}{k_B T_1}\right)$$

And the backward jumping rate (due to the action of the ratchet spring at T_2) is:

$$R_- = R_0 \exp\left(-\frac{E + \tau\theta}{k_B T_2}\right)$$

3. Average velocity

The average angular velocity is given by:

$$\langle \omega \rangle = \delta\theta \cdot (R_+ - R_-)$$

where $\delta\theta = \frac{2\pi}{N}$ is the angle per tooth.

4. Condition for useful work

The system performs work ($\langle \omega \rangle > 0$ and $\tau > 0$) only if:

$$\frac{R_+}{R_-} = \exp\left[\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \cdot \frac{\tau\theta}{k_B}\right] > 1$$

That is, if $T_1 > T_2$, the system can rotate preferentially in one direction and extract work from the thermal gradient. If $T_1 = T_2$, there is no net motion: the second law is fulfilled.

5. Energy balance

The useful extracted power is:

$$P = \tau \langle \omega \rangle$$

And the heat flux comes from the hot gas:

$$\dot{Q}_{T_1} = R_+ E - R_- E$$

6. Conclusion

The system works as a heat engine only if $T_1 > T_2$. It cannot extract useful work from a single thermal bath, confirming the second law of thermodynamics.

Appendix: Generalized Szilard Engine and the Landauer Principle

Introduction: Explanation of the principles and the engine

To understand this, we will assume another thought experiment.

We consider a particle in a box of a certain volume V , with a bath at temperature T . We begin a cyclic process:

1. We measure the side where the particle is.
2. We insert a piston with no energy cost that divides the box into two halves of volume $V/2$.
3. We perform a quasi-static isothermal expansion and the piston is pushed by the particle until the volume V is recovered.

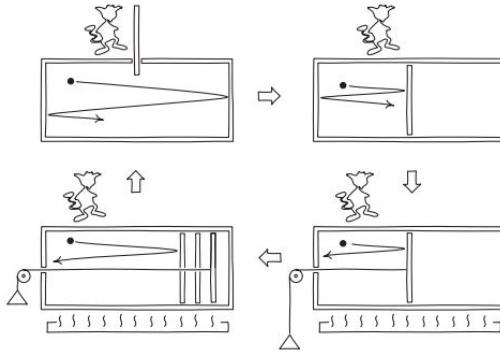


Figure 1: Diagram of the Szilard engine or machine. A barrier is introduced in the middle of the box and is displaced quasi-statically by the particle, obtaining information about where it is. This introduces the idea that information is equivalent to a minimum work. Image belonging to [7]

The equation that governs the work produced

by the expansion of the piston at constant T is:

$$W = \int_{V/2}^V k_B T \frac{dV'}{V'} = k_B T \ln 2 \quad (1)$$

If it were repeated infinitely many times, it would seem to violate the second law. This process represents the Szilard model.

This process can be modelled in other ways. The partition of the volume when inserting the piston may be greater or less than $V/2$ and a quantum version of the model can even be made, but even so the same conclusion is recovered: information has an energetic value. By assuming a massless piston, with an apparently simple model in which we consider the restoration of the initial state in a quasi-static way, work is performed simply due to the fact of knowing a certain physical information.

This raises a series of questions: Does measurement produce entropy? Does recording information have an intrinsic and minimum energetic cost? If it does, is it in the storage or in the erasure of information?

As we have seen, the initial and final states are identical, which means that there is no change in free energy in the system, which would imply that the system extracts work from the reservoir in each cycle, thus violating the second law. To be fully rigorous, this work would have a negative sign by convention, since it is extracted from the heat bath.

Here is where the Landauer principle comes into play. We assume that there is a physical system that can store the information about the state of the particle, whether it is on the left or on the right, and act accordingly. We thus form a memory-meter set. Each state represents one bit of information and the memory is a physical two-state system in correspondence with the two possible states of the box, which is reflected in the memory. To repeat the cycle after the first measurement and isothermal expansion, that memory should be erased, otherwise one cannot know where the particle is now, since it is the memory of the previous case but not of the current one. This erasure action involves “restoring” the

memory to a neutral state that is neither of the two corresponding to the box.

$$W_{\text{erasure}} \geq k_B T \ln 2 \quad (2)$$

Since it is precisely this erasure action that is worth at least one bit of energy, which can be dissipated in the form of heat, work...

$$Q \geq k_B T \ln 2 \quad (3)$$

This minimum does not depend on the Szilard engine, but on eliminating a bit of uncertainty in general in physics. It is a minimum quantity in thermodynamics and statistical physics.

In this way, as a limiting case,

$$W_{\text{total}} = -k_B T \ln 2 + k_B T \ln 2 = 0 \quad (4)$$

Where in reality, the work will be larger in practice due to energy dissipation in the erasure of the memory. This can be applied to entropy and, in conclusion, the total entropy will not decrease when considering all the physical systems involved, thus preserving the second law.

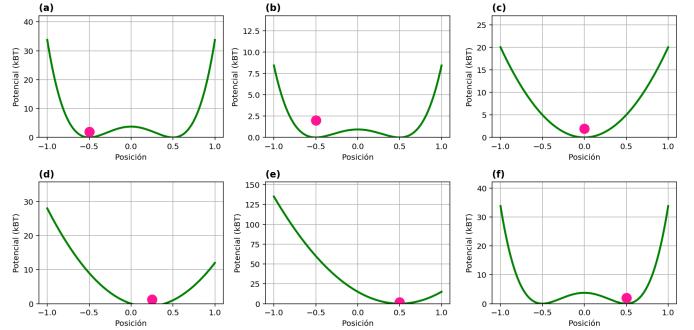


Figure 2: Schematic sequence of the process of erasing one bit of information, illustrated through the progressive deformation of a double-well potential within the framework of the Landauer principle. Subfigures (a) to (f) represent different moments of this process, ordered from left to right. In (a), the potential is symmetric and presents two stable minima, which represent the two possible logical states of the bit (0 in the left minimum and 1 in the right minimum); the particle (pink dot) can be found in either of them, which corresponds to a situation of maximum uncertainty (1 bit of information). In (b), an asymmetry is introduced that begins to favour state 0, tilting the potential towards the left minimum. In (c), the right minimum has been raised until it becomes unstable, and the particle inevitably migrates to the left side. In (d) and (e), the system has been forced into a single energy minimum (corresponding to bit 0), which constitutes the physical erasure of the information. Finally, in (f), the potential becomes symmetric again, but the particle remains in the left minimum: the bit has been reinitialized in state 0, with total loss of the previous information. According to the Landauer principle, this process implies a minimum dissipation of energy of $k_B T \ln 2$ as a consequence of the destruction of information.

In short, any physical system capable of storing information from a measurement dissipates a minimum amount of energy applied to erase that information in order to perform a cyclic process. Information has an energetic cost through mem-

ory erasure.

Generalized engine

1. Configuration and phases of the engine

A one-dimensional box of length L is considered, in which a partition is inserted at a position $L_x \neq \frac{L}{2}$. A classical ideal gas (a single particle) is initially in thermal equilibrium at temperature T with a thermal reservoir.

The process consists of the following phases:

1. **Insertion of the partition:** without work or heat exchange (ideal process).
2. **Measurement:** it is determined on which side the particle is (left or right).
3. **Quasi-static expansion:** the particle is allowed to push the partition to a new equilibrium position L_x^* , extracting work.
4. **Removal of the partition:** again ideal.

2. Probabilities and entropy

The probability that the particle is on the left after inserting the partition at L_x is:

$$P_L = \frac{L_x}{L}, \quad P_R = \frac{L - L_x}{L}$$

The Shannon entropy associated with the measurement is:

$$S_{\text{info}} = -k_B(P_L \ln P_L + P_R \ln P_R)$$

3. Extracted work

If the partition is allowed to move quasi-statically to a new equilibrium position L_x^* , the average extracted work is:

$$\langle W \rangle = k_B T \left[P_L \ln \left(\frac{L}{L_x} \right) + P_R \ln \left(\frac{L}{L - L_x} \right) \right]$$

This expression reduces to the well-known $W = k_B T \ln 2$ in the symmetric case $L_x = \frac{L}{2}$.

4. Application of the Landauer principle

Reading the position of the particle does not require energy, but erasing the memory does.

According to the **Landauer principle**, erasing one bit of information with entropy S_{info} entails a minimum heat dissipation:

$$Q_{\text{diss}} \geq TS_{\text{info}} = -k_B T(P_L \ln P_L + P_R \ln P_R)$$

5. Recovery of the second law

The net entropy balance considering the system and the environment (including the erasure of information) is:

$$\Delta S_{\text{total}} = -\frac{\langle W \rangle}{T} + \frac{Q_{\text{diss}}}{T} \geq 0$$

This ensures that the second law is not violated: any gain of work from information must be accompanied by an equal or greater dissipation in the environment.

6. Equilibrium case of the piston

The equilibrium position of the piston L_x^* is determined by equal pressure on both sides. For a single particle, this is equivalent to maximizing the entropy:

$$P_L \cdot \ln \left(\frac{L_x^*}{L_x} \right) + P_R \cdot \ln \left(\frac{L - L_x^*}{L - L_x} \right) = 0$$

Solving for L_x^* , one finds that the final position depends on L_x , reflecting the bias introduced by the asymmetric partition.

Appendix: Quantum Szilard engine and informational demons

This appendix explains the case proposed by the authors of “A friendly guide to exorcise Maxwell’s Demon”.

1. The quantum Szilard engine

We consider a quantum version of the Szilard engine, where a quantum particle is in a one-dimensional box of length L , with an infinite potential at the ends. The system is analysed at finite temperature, which introduces relevant thermal and statistical effects.

- In the classical case, by inserting a piston in the middle ($x = L/2$), work can be obtained when expanding it after a position measurement.
- In the quantum case, the change of the energy level spectrum before and after inserting a barrier is considered. The energy of the ground state changes depending on the symmetry of the wave function.

2. Quantum states and entropy

The thermal state of the system is described by the density matrix:

$$\rho = \frac{1}{Z} \sum_n e^{-\beta E_n} |n\rangle\langle n|$$

where $Z = \sum_n e^{-\beta E_n}$ is the partition function and $\beta = 1/(k_B T)$. The von Neumann entropy associated with the thermal state is:

$$S = -k_B \text{Tr}(\rho \ln \rho)$$

3. Barrier insertion and energy change

When inserting a barrier at $x = L/2$ in the quantum case, the system is divided into two wells. The even wave functions are not affected, but the odd ones are. This induces a change in the spectrum:

$$\Delta E = E_n^{\text{post}} - E_n^{\text{pre}}$$

where the energies can be calculated as a function of the length of each sub-box.

The maximum work extracted after the measurement is:

$$W_{\text{extracted}} = k_B T \ln 2$$

if the wall is placed exactly in the middle.

4. Generalized case: partition at L_1 and L_2

If the wall is not inserted at $L/2$, but at an arbitrary position, the maximum extracted work is generalized as:

$$W = k_B T \ln \left(\frac{L_1}{L_2} \right)$$

where L_1 is the side where the particle is located after the measurement.

5. The role of the demon and the Landauer principle

To close the thermodynamic cycle without violating the second law, the demon must erase the information acquired upon measuring. This erasure has a minimum energetic cost (Landauer principle):

$$W_{\text{erasure}} \geq k_B T \ln 2$$

This exactly compensates the work obtained from the system, restoring the validity of the second law:

$$\Delta S_{\text{total}} \geq 0$$

6. Interpretation

This scheme shows that even in quantum contexts, the use of information to extract work does not contradict thermodynamics as long as the cost of processing and storing information is properly accounted for.

Reference of this appendix:

- A. C. Elouard, M. Richard, and A. Auffèves, "A friendly guide to Maxwell's demons" (2023)

Anexo de gráficas

