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Dynamic Cooling of multiple qubits

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Contents

Introduction iii

1 Basics of Quantum Thermodynamics 1
- 1.1 Thermodynamics . . . 1
  - 1.1.1 Energy and Entropy: the Laws of Thermodynamics . . . 3
- 1.2 Quantum Theory . . . 5
  - 1.2.1 The Postulates of Quantum Mechanics . . . 5
  - 1.2.2 Density Matrix . . . 6
- 1.3 Work, Heat and the First law . . . 8
  - 1.3.1 Quantum Work . . . 8
  - 1.3.2 Heat and the first Law . . . 10
- 1.4 Entropy and the Second law . . . 12
  - 1.4.1 Entropy and Information . . . 13
  - 1.4.2 The Second Law . . . 14
- 1.5 Equilibrium . . . 16
  - 1.5.1 Jaynes principle . . . 16
  - 1.5.2 Thermalization . . . 19
- 1.6 The Zeroth and the Third law . . . 20
  - 1.6.1 The Zeroth Law . . . 20
  - 1.6.2 The Third Law . . . 21
- 1.7 Maximal Work Extraction . . . 21

2 Quantum Thermodynamics for Quantum Computing 23
- 2.1 Quantum Computation . . . 24
  - 2.1.1 Quantum Bits, Quantum Circuits . . . 24
  - 2.1.2 Quantum Algorithms . . . 28
  - 2.1.3 Requirements for Quantum Computation . . . 30
- 2.2 Algorithmic Cooling . . . 31
  - 2.2.1 Closed system . . . 32
  - 2.2.2 Heat Bath Algorithmic Cooling . . . 34

2.3 Dynamic Cooling 35
2.3.1 Optimal Unitaries 35
2.3.2 Cooling Temperature 37
2.3.3 Estimates for the Temperature 40
2.4 Dynamic Cooling with non-identical machine qubits 42
2.4.1 3 qubits example 42
2.4.2 General Case: Fundamental inequalities for permutations 44
2.4.3 Application: Identical qubits 47

3 Single shot cooling of multiple qubits **49**
3.1 Unitaries for identical qubits 49
3.1.1 Optimal Unitaries 50
3.2 On the unique temperature condition 55
3.2.1 Solutions for the Partition Problem 55
3.2.2 Off diagonal terms restore unique temperature 59
3.3 Cooling Temperature 67
3.3.1 Two target qubits 67
3.3.2 M target qubits 70
3.3.3 Estitmate for $\xi_M^\star$ 73

Conclusions **76**

Introduction

Quantum computers offer the potential advantage of solving specific problems with exponential efficiency, compared to classical ones. At the same time, they are extremely delicate systems, and to guarantee faithful performances, they have to be isolated from the environment in order to reduce errors. This is done through the cooling of the quantum computer: the system is positioned in a highly controlled environment in which the temperature is decreased thanks to techniques such as dilution refrigerators or laser cooling. However, this is not enough. It is also necessary that qubits are initialized: this translates into the requirement that the initial state be a "pure state", set with certainty in the logical state 0...0. From a thermodynamic perspective, this corresponds to the task of cooling a quantum system to its ground state, a problem that is well known in Thermodynamics for its impossibility: the third principle of Thermodynamics. Indeed, this is also called "the unattainability principle", since it postulates that infinite resources are required to cool a system to its ground state. Thus, to guarantee reliable quantum computation, a central problem becomes that of cooling as much as possible a quantum system given finite resources.

In this work, we use the framework of Quantum Thermodynamics to answer a specific problem in initialization: given a closed quantum system composed of N qubits with equal temperature T and a number M of desired qubits, is it possible to cool these M qubits at a lower temperature T'? What is the minimum temperature possible?

With the aim of formulating these problems in the correct mathematical terms, in Chapters 1 and 2 we introduce the necessary prerequisites.

Since the task is to cool qubits, we need to place the theory of Thermodynamics in the correct framework, which is that of quantum mechanics: this is done in Chapter 1, where the concepts of heat and work acquire a proper quantum

mechanical meaning. In particular, the chapter is focused on closed quantum system Thermodynamics, and much emphasis is given in the strict connection between Thermodynamics and the theory of information. A first important result that we show is the description of thermal state as the Gibbs state: this is proven thanks to "Jaynes Principle", which, particularly, connects equilibrium states with maximum entropy. This, together with the ETH hypothesis, guarantees the accuracy of describing a finite quantum system at thermal equilibrium as a Gibbs state. Since the initial system under examination is a thermal equilibrium state of N qubits, Jaynes and the ETH enable us to mathematically describe it in the form of Gibbs. In the end of the chapter, two crucial results are introduced. The first is the "Third Principles of Thermodynamics", which constitutes the first fundamental limitation to the amount of cooling that we can perform on a quantum system, and the second in the concept of "Ergotropy". This represents the maximal amount of work that can be extracted from a quantum system, and is of crucial importance for cooling: by considering the initial N qubits as a bipartite system target plus ancilla $T + A$ (with "target" as the qubits to be cooled and "ancilla" as resource qubits) we can use ergotropy to extract energy from the target, decreasing their temperature at the cost of the ancilla's system.

In Chapter 2, the focus is shifted to the quantum computing side of the problem. After the introduction of qubits and gates, the problem of initializing qubits is addressed. Following an historical path, we start with the first proposals on cooling qubits through quantum algorithms. This practically means that an initial ensemble of qubits undergoes a unitary operation, which separates the system into two regions: that of target qubits, which becomes cold, and that of the ancillas, which becomes hot. In this context, the unitary operator acts as an entropy compression, which absorbs the entropy of the target to pump it into the ancillas: this process is naturally bounded by Shannon's limit, which imposes a constraint on the amount of entropy that can be extracted from a subsystem, since the total entropy of the closed system must be conserved. This naturally leads to the introduction of open system dynamics in order to overcome Shannon's bound. However, this will be just mentioned: our scope is the study of closed systems, and for this reason we end the chapter with the exposition of two closed system dynamics scenarios. In the first, N identical qubits undergo the unitary operation such that as output 1 qubit is cooled at the expense of the others, while in the second the same task is dealt with by starting with N non-identical qubits. The former is the one on which all our interests have been focused, as the objective of our work is the generalization of the process for arbitrary M qubits.

Lastly, Chapter 3 represents the core of our original work. In it, we finally set the question introduced before in the correct mathematical terms. The analysis yields several non-trivial results.
In the first place, the fact that the target system is made of $M > 1$ qubits means that we have an additional constraint on the unitary operator, which is that of maintaining the temperature of target qubits the same between each other - their density matrices must be locally identical. This has been translated into a condition on the density matrix of the ancillas that a correct ordering must guarantee, and practically translates into a highly sophisticated partitioning problem. It turns out that a solution to this problem does not always exist: a first important result concerns the feasibility of building a unitary operator for a given couple (N, M).
Moreover, we also provide a workaround when this condition cannot be fulfilled: we show that, by symmetry arguments, mixing the eigenvalues through a Quantum Fourier Transform, we can recover a final state for which local qubits have an identical temperature. However, this comes at the cost of introducing off diagonal terms between particular subspaces of the final state.
Finally, we address the second central question of this work and derive a low-temperature estimate for the minimum achievable target temperature, expressed as a simple formula connecting T, N and M.

Chapter 1

Basics of Quantum Thermodynamics

The term 'Thermodynamics' derives from the Greek words therme ('heat') and dynamis ('power'), reflecting the discipline's historical roots in harnessing the power of heat to perform work. Indeed, Thermodynamics is the branch of physics that deals with work, heat, and energy. While it originated with the goal of improving the efficiency of steam engines, the theory proved to be remarkably general, with consequences that extend far beyond the optimization of thermal machines, leading to question the nature of time, the evaporation of black holes, and the fate of the universe.
In this chapter, we introduce the theory of quantum Thermodynamics, following the lecture notes [1–3]. We start by recalling the principles of standard Thermodynamics in Section 1.1, and we build the theory in the quantum setting in the following sections. In particular, we derive and reinterpret thermodynamical principles in light of quantum mechanics, which is rapidly recalled in Section 1.2, starting from the first principle (Section 1.3), entropy and equilibrium (Sections 1.4-1.5), to the zeroth and the third principles (Section 1.6). In the last section (Section 1.7), we deal with the problem of maximizing work extraction from a quantum system, a task that is of crucial importance for our work.

1.1 Thermodynamics

In real conditions, to rigorously predict the behavior of a steam engine is an incredibly difficult task, especially if we consider the state of technology in the early 19th century: it is far more effective to focus on a small set of macro-

scopically emergent quantities - referred to as "thermodynamic variables", for example the Pressure "P", the Temperature "T" or the Volume "V" - and to study how they relate to each other when the steam engine is in a stationary condition. This means that, once the machine is running, we wait until its behavior becomes time-independent, and only from that moment on we start to slightly change the parameters under observation. Hidden within this scenario are two key features of the theory of standard Thermodynamics: the concept of equilibrium and the assumption of quasistatic processes.
We define equilibrium as the condition under which the thermodynamic variables remain constant over time. Moreover, we introduce the first important principle in Thermodynamics, which states how thermodynamic systems in equilibrium relate to each other.

Zeroth Law of Thermodynamics: if two systems A and B are in equilibrium with a third system C, then A is in equilibrium with B.

In this context, the statement "A is in equilibrium with B" means that both A and B are in equilibrium when placed in thermal contact with each other. In mathematical terms, states that are in thermodynamic equilibrium with each other form an equivalence class in the total configuration space.

Moreover, the relation between the thermodynamic variables at equilibrium can be represented by a function of the variables themselves, which is called equation of state:

$$f(P,V,T)=0. \tag{1.1}$$

The equation of state defines the manifold of equilibrium states $\mathscr{M}$. Quasistatic processes are those in which the system remains at equilibrium at all instants, and are thus described by paths in the manifold of equilibrium states. Precisely, the process $\mathscr{P}(t)$, which takes place between time t_0 and time t_1, is a curve s.t.

$$\mathscr{P}(t)\in\mathscr{M},\ \forall\ t\in[t_0,t_1].$$

In the absence of dissipations, quasistatic processes are reversible. Irreversible processes are then defined as $\mathscr{P}_i(t)$ such that

$$\exists t \text{ s.t. } \mathscr{P}_i(t)\notin\mathscr{M}.$$

A more intuitive representation is provided in Figure 1.1. Note that there is a core contradiction in the formulation of standard Thermodynamics: since equilibration takes an infinite amount of time to occur, it is not mathematically possible to have a finite-time reversible process. However, since practically the exponential of equilibration will arrive at regime with relaxation time $\tau<\infty$, with τ negligible with respect to the time scale of the system under exam, this description holds at first approximation.

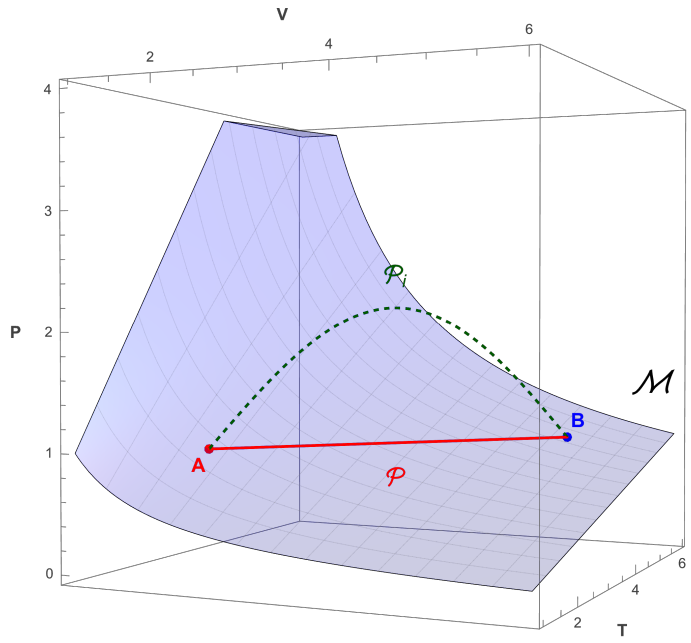

Figure 1.1: Conceptual representation of a thermodynamic manifold $\mathscr{M}$. In red, a reversible process between the points A and B is drawn, while the green dotted line represents an irreversible process between the same points.

1.1.1 Energy and Entropy: the Laws of Thermodynamics

In the spirit of classical mechanics, the first quantity that we analyze is energy. In steam engines, the goal is to produce work. This comes at the expense of producing a different form of energy: heat. This describes the worst form of energy - the one that is dissipated during a process and is not convertible into work. In the following, we describe work with the letter W and heat with Q. If we can extract work from a system, then it is already associated with some form of energy. This is the internal energy, and we describe it with U. The relation that connects these three forms of energies is given by the following Law.

First Law of Thermodynamics:

$$\Delta U = \Delta W + \Delta Q, \tag{1.2}$$

where, by convention, we take $W > 0$ if it is done on the system, and $Q > 0$ if it flows in the system. More precisely, the law can be expressed in its differential form:

$$dU = \delta W + \delta Q, \tag{1.3}$$

where the local nature of the energies is specified: dU is an exact differential, i.e. it does not depend on the path taken from one point of the manifold to another, but only on the end points of the process. On the other hand, δW and δQ are inexact differentials: their integral depends on the path taken.
It is relatively easy to show that the work can be written as a function of an exact differential

$$\delta W = -PdV, \tag{1.4}$$

where P is the thermodynamic pressure. At this point, one might wonder if there is a similar relation for heat δQ: the answer is yes, and it is provided by Clausius [4]. In his work, he found the so called "Clausius inequality"

$$\oint \frac{\delta Q}{T} \leq 0, \tag{1.5}$$

which, for reversible processes, becomes an equality. This means that $\delta Q/T$ is an exact differential, called thermodynamic entropy:

$$dS := \frac{\delta Q}{T}. \tag{1.6}$$

This fact automatically leads to an important result. Indeed, consider an irreversible process from state A to state B, then followed by a reversible one from B to A:

$$\oint \frac{\delta Q}{T} = \int_A^B \frac{\delta Q}{T} + \Delta S_{B\to A} = \int_A^B \frac{\delta Q}{T} - \Delta S_{A\to B} \leq 0, \tag{1.7}$$

where we used, for reversible processes, $\Delta S_{A\to B} = -\Delta S_{B\to A}$. This means that

$$\int_A^B \frac{\delta Q}{T} \leq \Delta S_{A\to B}, \tag{1.8}$$

which, since for isolated systems $\delta Q = 0$, gives the following result.

Second Law of Thermodynamics: the Entropy of the universe (as system plus environment, $S + E$) is a non-decreasing function

$$\Delta S = \Delta S_S + \Delta S_E \geq 0. \tag{1.9}$$

Although for an isolated system $S+E$, the only effect of a process is the increase in total entropy, we must clarify that entropy can decrease for systems that are not isolated. For example, considering only the system S, which couples to E to form the isolated system $S + E$, it is possible that its entropy decreases:

$\Delta S_S < 0$. In that case, a decrease in entropy implies a greater increase of entropy in the systems to which it is coupled, to guarantee the validity of Equation 1.9: $\Delta S_E \geq |\Delta S_S|$.
The Second Law constitutes a fundamental result: it enables us to distinguish which processes spontaneously occur in nature and sets a constraint on the efficiency of thermal machines. Moreover, it is the first physical law that presents an asymmetry in the time direction. Indeed, all isolated physical systems evolve by increasing their entropy until they reach thermal equilibrium: eventually, this is conjectured to occur to the universe itself, causing its "heat death".

1.2 Quantum Theory

As the objective of this chapter is to set Thermodynamics in a quantum framework, it is not possible to do so without introducing the core principles of the theory first.

1.2.1 The Postulates of Quantum Mechanics

The mathematical framework is set through the postulates.

Postulate 1: any isolated system S is associated with a Hilbert space $\mathscr{H}_S$, which is a complete vector space with norm induced by the scalar product. The state of the system is described by a unit vector $|\psi\rangle \in \mathscr{H}_S$.

Postulate 2: the evolution of a closed system is described by means of a unitary operation $\mathscr{U}$, such that

$$|\psi(t)\rangle = \mathscr{U}(t)\,|\psi(0)\rangle\,. \tag{1.10}$$

The specific form of $\mathscr{U}$ is given by solving the Schrödinger equation

$$i\hbar\frac{d\,|\psi\rangle}{d\,t} = H\,|\psi\rangle\,, \tag{1.11}$$

where H represents the Hamiltonian operator.

Postulate 3: measurements of the state of the system S are described by operators M_m acting on the state space $\mathscr{H}_S$. The index "m" refers to the measurement outcome that could occur and the probability of obtaining it is:

$$p(m) = \langle\psi|\,M_m^\dagger M_m\,|\psi\rangle\,. \tag{1.12}$$

After the measurement, the state $|\psi\rangle$ collapses onto the state:

$$\frac{M_m |\psi\rangle}{\langle\psi| M_m^\dagger M_m |\psi\rangle}. \tag{1.13}$$

Moreover, the normalization of probabilities $\sum_m p(m) = 1$ induces a property on the measurement operators:

$$\sum_m M_m^\dagger M_m = \mathbb{1}, \tag{1.14}$$

where $\mathbb{1}$ is the identity operator.

Postulate 4: the system S given by the composition of N systems s_i has a state space $\mathscr{H}_S$ given by the tensor product of the subsystem state spaces $\mathscr{H}_{s_1} \otimes \mathscr{H}_{s_2} \otimes \mathscr{H}_{s_1}$..., such that

$$\mathscr{H}_S = \bigotimes_{i=1}^{N} \mathscr{H}_{s_i}. \tag{1.15}$$

Moreover, if the state of each subsystem is $|\psi_i\rangle$, then the state of the total system S is the tensor product:

$$|\psi\rangle = \bigotimes_{i=1}^{N} |\psi_i\rangle. \tag{1.16}$$

1.2.2 Density Matrix

In real experiments, it is rare to have complete knowledge of a quantum system. It is much more likely to know that the system is in state $|\psi_i\rangle$ with some probability p_i. This is the main intuition that lead von Neumann and Landau to the introduction of a new quantity, which became known as "Density Operator" (or "Density Matrix").

Suppose that we are dealing with a quantum system that is in the state $|\psi_i\rangle$ with probability p_i. We define the density operator of this system as

$$\rho := \sum_i p_i |\psi_i\rangle \langle\psi_i|. \tag{1.17}$$

From the definition, we have the following properties:

$$\begin{aligned}
\mathrm{Tr}[\rho] &= \mathrm{Tr}\left[\sum_i p_i |\psi_i\rangle \langle\psi_i|\right] = \sum_i p_i \mathrm{Tr}[|\psi_i\rangle \langle\psi_i|] = \sum_i p_i = 1, \\
\langle\phi|\rho|\phi\rangle &= \sum_i p_i \langle\phi|\psi_i\rangle \langle\psi_i|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0, \\
\rho^\dagger &= \sum_i p_i^\dagger (|\psi_i\rangle \langle\psi_i|)^\dagger = \sum_i p_i |\psi_i\rangle \langle\psi_i| = \rho,
\end{aligned} \tag{1.18}$$

where we used the ciclicity of the trace, the normalization condition of the probabilities p_i and the fact that $p_i \in \mathbb{R}_{[0,1]}$.
Thus, the density matrix is an operator that is Hermitian, positive, and with unit trace.

Moreover, is easy to generalize the features of the state vector to the density matrix.

Evolution: since the state vector evolves as $|\psi'\rangle = U|\psi\rangle$, for the density matrix ρ we have

$$\rho' = \mathscr{U}\rho\mathscr{U}^\dagger, \tag{1.19}$$

as can be easily checked by the definition of ρ.

Expectation Values: given an Hermitian operator O, its expectation value for the system described by ρ is given by:

$$< O >= \mathrm{Tr}[O\rho]. \tag{1.20}$$

Measurements: the action of the measurement operator M_m on ρ would give the outcome "m" with probability

$$p(m) = \mathrm{Tr}\left[M_m^\dagger M_m \rho\right], \tag{1.21}$$

with the post measurement state collapsing onto

$$\frac{M_m \rho M_m^\dagger}{\mathrm{Tr}\left[M_m^\dagger M_m \rho\right]}. \tag{1.22}$$

Composite States: the state ρ_S given by the composition of N states ρ_{s_i} is given by their tensor product:

$$\rho_S = \bigotimes_{i=1}^{N} \rho_{s_i}. \tag{1.23}$$

It turns out that all the postulates introduced in the language of the state vector $|\psi\rangle$ can be rewritten in the more general framework of the density operator, which loses its ensamble interpretation and becomes the true description of the quantum state.

Before delving into the description of thermodynamic phenomena, we need to add one last crucial definition: the partial trace.

Indeed, while we treated the trivial case in which we start from subsystem states ρ_{s_i} to find the total state ρ_S that contains all subsystems, the case in which we start from a total state ρ_S and we want to find a particular subsystem state was left unanswered.

The tool that allows us to perform that operation is that of the Partial Trace: consider the bipartite system $\mathscr{H} = \mathscr{H}_a \otimes \mathscr{H}_b$ with state ρ, we can find the state of the subsystem "a" as

$$\rho_a = \mathrm{Tr}_b[\rho] := \sum_\beta \langle\beta|\rho|\beta\rangle, \tag{1.24}$$

with $\{|\beta\rangle\}$ an orthonormal basis of $\mathscr{H}_b$.

Equipped with this definition, we can finally try to understand thermodynamic phenomena through the language of quantum mechanics.

1.3 Work, Heat and the First law

The derivation of thermodynamic quantities in the framework of quantum mechanics starts with the search for the definition of work and heat.

1.3.1 Quantum Work

We start our analysis by focusing on closed quantum systems, i.e. systems that evolve through a unitary dynamics generated by a time dependent Hamiltonian $H = H(\lambda)$, where $\lambda = \lambda(t)$ is a control parameter that depends on time. In analogy with standard Thermodynamics, the most relevant quantity for such a system is given by its internal energy:

$$U(t) = \mathrm{Tr}[H(\lambda(t))\rho(t)]. \tag{1.25}$$

Notice that, by accounting for possible time dependent density matrices $\rho(t)$, this definition holds also for non-equilibrium Thermodynamics. The crucial

observation here is that the system evolves unitarily and, as such, the *Von Neumann entropy* $S(\rho) = -\mathrm{Tr}[\rho \log(\rho)]$ (see Section 1.4) does not change with time: we can only interpret the energy difference as mechanical work

$$W(t) = \mathrm{Tr}[H(t)\rho(t)] - \mathrm{Tr}[H(0)\rho(0)] = U(t) - U(0) = \Delta U(t). \tag{1.26}$$

In analogy with standard Thermodynamics, we can rewrite the work as a differential form:

$$\begin{aligned} W(t) &= \int_0^t dt' \frac{d}{dt'} \mathrm{Tr}\big[H(t')\rho(t')\big] = \\ &= \int_0^t dt' \left\{ \mathrm{Tr}\left[\left(\frac{d}{dt'}H(t')\right)\rho(t')\right] + \mathrm{Tr}\left[H(t')\left(\frac{d}{dt'}\rho(t')\right)\right]\right\} = \\ &= \int_0^t dt' \delta W. \end{aligned} \tag{1.27}$$

The second term in the second line vanishes, as one can easily prove by using Liouville-Von Neumann equation $i\hbar\dot{\rho} = [H, \rho]$ and the cyclicity of the trace. Thus, we define the work as

$$\delta W(t) := \mathrm{Tr}\left[\left(\frac{d}{dt}H(t)\right)\rho(t)\right], \tag{1.28}$$

which by convention is the work done on the system.

It is easy to generalize the notion of work for composite systems. Consider a composite quantum system whose Hilbert space is the tensor product of two

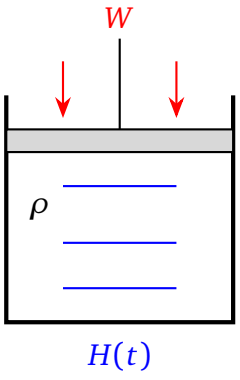

Figure 1.2: Analogy with the scenario of standard Thermodynamics: a closed cylinder represents the closed quantum system ρ, the moving piston above it represents the work done on the quantum system.

systems S and E, which models a system coupled to an external environment: $\mathscr{H}_s \otimes \mathscr{H}_e$, where the subscript "$e$" refers to "environment". Since the systems are not isolated from each other, they will exhibit interactions. Thus, the total Hamiltonian is:

$$H(t) = H_s(t) \otimes \mathbb{1}_e + \mathbb{1}_s \otimes H_e + H_{se}(t), \tag{1.29}$$

where we implicitly assumed that the time dependence of the interaction term is only induced in the system Hamiltonian, and not in the environment. Using Equation 1.28 with the total Hamiltonian $H(t)$ gives us

$$\delta W(t) = \mathrm{Tr}_{se}\left[\left(\dot{H}_s(t) \otimes \mathbb{1}_e\right)\rho_{se}(t)\right] + \mathrm{Tr}_{se}\left[\dot{H}_{se}(t)\rho_{se}(t)\right], \tag{1.30}$$

from which we can trace out the environment in the first term, obtaining

$$\delta W(t) = \mathrm{Tr}_s\left[\frac{dH_s(t)}{dt}\rho_s(t)\right] + \mathrm{Tr}_{se}\left[\frac{dH_{se}(t)}{dt}\rho_{se}(t)\right]. \tag{1.31}$$

This represents the (inexact) differential of the work done on the total system.

1.3.2 Heat and the first Law

In standard Thermodynamics, there is another quantity that describes a form of energy: heat. Heat is classically seen as a disordered form of energy, and it is the one that is inevitably lost in the environment.
In the quantum setting, we define it, again, starting from the total energy. Consider, as before, a composite system made of a quantum system coupled to the environment. The internal energy differential in this context is

$$dU = \frac{d}{dt}\mathrm{Tr}\left[H(t)\rho_{se}(t)\right], \tag{1.32}$$

where $H(t)$ is defined by Equation 1.29. We can split the equation by letting the time derivative operate separately on the Hamiltonian and on the density matrix. We find

$$\begin{aligned} dU = \mathrm{Tr}\left[\frac{d}{dt}(H_s(t) \otimes \mathbb{1}_e + \mathbb{1}_s \otimes H_e + H_{se}(t))\rho_{se}(t)\right] + \\ + \mathrm{Tr}\left[(H_s(t) \otimes \mathbb{1}_e + \mathbb{1}_s \otimes H_e + H_{se}(t))\frac{d}{dt}\rho_{se}(t)\right], \end{aligned} \tag{1.33}$$

We can separate the contributions related to the system and the environment, and we obtain

$$dU = \delta W(t) + \delta\tilde{Q}_s + \delta\tilde{Q}_e + \mathrm{Tr}_{se}\left[H_{se}(t)\frac{d\rho_{se}(t)}{dt}\right], \tag{1.34}$$

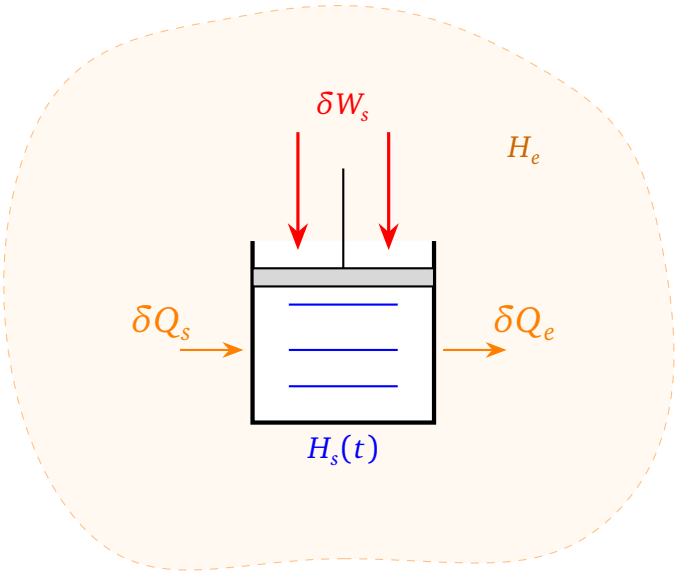

Figure 1.3: Generalisation of previous scenario for a composite system. Here the presence of the environment enables heat flow between system and bath and viceversa. Notice that in this representation we would not be able to draw a correct representation of the interactive terms containing H_{se}, since their nature is not clear.

where $\delta\tilde{Q}_i := \mathrm{Tr}_i[H_i(t)\dot{\rho}_i(t)]$ represents an energy contribution given by the change in the density matrix of separate subsystems. This equation makes evident a major problem in quantum Thermodynamics: the presence of a non-negligible term H_{se} does not allow to separate terms between the system and the environment. In fact, it is still not well understood how this form of energy should be shared between the degrees of freedom at play, nor it is understood if it should be interpreted as work or heat. A regime in which these problems disappear is that of the weak-coupling: suppose that the interaction Hamiltonian term H_{se} is negligible compared to the energies of system and environment. Defining the thermodynamic heat as

$$\delta Q := \mathrm{Tr}\left[H(t)\frac{d}{dt}\rho(t)\right], \tag{1.35}$$

which is taken as positive when it enters the system, we get, for the total energy differential, $dU = \delta W + \delta Q_s + \delta Q_e$. For the subsystem S:

$$dU_s = \delta W_s(t) + \delta Q_s, \tag{1.36}$$

where U_s is the internal energy of the subsystem S, and W_s and Q_s are the work done on the system S and the heat flowing into S. This equation correctly reproduces the First Law of Thermodynamics.
Note that, when the environment is composed of multiple baths, we have $\delta Q = \sum_\alpha \delta Q_{\beta_\alpha}$.

1.4 Entropy and the Second law

Entropy is one of the most famous concepts in Physics, and probably among those most frequently misunderstood. As mentioned in Section 1.1, it was introduced to express heat as a function of an exact differential, but now its meaning lies within the theory of information.
In its original form, it was interpreted as a measure of the energy that cannot be turned into work and, at the same time, as a measure of irreversibility. It was with the atomic hypothesis and the formulation of statistical mechanics that entropy acquired a more detailed meaning. Indeed, Boltzmann introduced the idea that Thermodynamics was the macroscopic consequence of the interaction of a huge number of particles (the so called "atoms"). In this setting, he interpreted entropy as a measure of the disorder of a thermodynamic system:

$$S = k_B \log(\Omega), \tag{1.37}$$

where k_B is the Boltzmann constant and Ω the number of microstates, i.e. the number of possible configurations that the system can have with the same

macroscopic properties. A more general formula is provided by the version of Gibbs:

$$S = -k_B \sum_i p_i \log(p_i), \tag{1.38}$$

which gives the entropy of those systems where microstates may not have equal probabilities. While developing the theory of information, Shannon found an identical mathematical expression to Equation 1.38, which became known as "Shannon entropy". This was the starting point of the interplay between information theory and statistical mechanics, which was later formalized by Jaynes [5, 6].

1.4.1 Entropy and Information

In information theory, effort is put into trying to understand how much informational content lies in some random event. For this scope, the first quantity we introduce is the Self Information.

Self Information: consider the random variable X that has the outcome x_j with probability p_j, the self information is given by

$$I_j := -\log(p_j). \tag{1.39}$$

This quantity can be intepreted as the surprisal of the occurrence of the outcome x_j: if $p_j = 1$ the surprise amounts to zero, while for $p_j \to 0$ the surprise diverges, as we did not expect the occurrence of that event. Taking the average self information, we find the most important quantity in information theory:

Shannon Entropy:

$$H(X) := -\sum_j p_j \log p_j, \tag{1.40}$$

which quantifies the average information gain when observing a random variable X, where the quantities p_j represent the probabilities of the occurrence of the result x_j. At the same time, it can be interpreted as the lack of information before measuring the variable X. Following the same steps, Von Neumann introduced the quantum version of entropy, which is given by the following definition.

Von Neumann Entropy: Consider a quantum system described by the density matrix ρ, which in its diagonal form is $\rho = \sum_j p_j |j\rangle \langle j|$; then the Von Neumann

Entropy is defined as

$$S(\rho) := -\mathrm{Tr}[\rho \log(\rho)] = -\sum_j p_j \log(p_j). \tag{1.41}$$

As its classical counterpart, it quantifies the lack of knowledge that we have on our quantum system: pure systems $\rho = |\psi\rangle\langle\psi|$ will have zero entropy, while the maximally mixed states $\rho = \mathbb{1}/d$ (with "d" dimension of the Hilbert space) have maximum entropy.
Generalizing existing quantities in classical information theory, we further introduce:

- *Quantum Relative Entropy*:
  Given two density matrices ρ and σ, we define

  $$\mathscr{D}(\rho||\sigma) := \mathrm{Tr}[\rho \log(\rho) - \rho \log(\sigma)], \tag{1.42}$$

  which quantifies the discrepancy in the entropy when we mistake a quantum state ρ with another σ. Note that the quantum relative entropy is a non-negative quantity, as is guaranteed by Klein's inequality

  $$\mathscr{D}(\rho||\sigma) \geq 0, \tag{1.43}$$

  with "=" iff $\rho = \sigma$.

- *Mutual Information*:
  Consider a bipartite system $\mathscr{H} = \mathscr{H}_a \otimes \mathscr{H}_b$, with $\rho_a = \mathrm{Tr}_b[\rho]$, $\rho_b = \mathrm{Tr}_a[\rho]$ and ρ density matrix of the total system. We define the mutual information as

  $$I(A:B) := \mathscr{D}(\rho||\rho_a \otimes \rho_b) = S(\rho_a) + S(\rho_b) - S(\rho). \tag{1.44}$$

  The mutual information tells us how much two systems are correlated with each other.

Now we have all the necessary equipment to derive the second principle in the framework of quantum mechanics.

1.4.2 The Second Law

The main feature of closed quantum systems is that they evolve unitarily. Among other things, this implies that the density matrix eigenvalues are conserved and consequently that the Von Neumann Entropy stays constant:

$$\partial_t S(\rho_{se}(t)) = \partial_t S(U(t)\rho_{se}(0)U^\dagger(t)) = 0. \tag{1.45}$$

This can be justified by reasoning on the fact that a closed system does not change its informational content, and for this reason the amount of information of the whole does not change with time. To quantify the informational evolution of the system, it is convenient to study the behavior of subsystems through another quantity, the *Entropy Production*[7].

Entropy Production

We introduce Entropy Production in standard Thermodynamics, and we later generalize to the quantum version. In standard Thermodynamics, it is well known (Section 1.1) that the entropy of a system S, placed in contact with N reservoirs at temperature T_i, is bounded by Clausius inequality

$$\Delta S_s \geq \sum_i \frac{Q_i}{T_i}, \tag{1.46}$$

where Q_i is the heat flowing into the system S from the reservoir "i" at temperature T_i. Based on this inequality, one introduces the entropy production as

$$\Sigma := \Delta S_s - \sum_i \frac{Q_i}{T_i} \geq 0. \tag{1.47}$$

In quantum Thermodynamics, we introduce entropy production with the following argument. Consider the variation of entropy of the subsystems composing the total system $S+E$, initially described by the factorized state $\rho(0) = \rho_s(0)\otimes\rho_e(0)$:

$$\Delta S_s(\tau) + \Delta S_e(\tau) = S_s(\tau) - S_s(0) + S_e(\tau) - S_e(0) = I(S(\tau) : E(\tau)), \tag{1.48}$$

where $I(S(\tau) : E(\tau))$ is the mutual information introduced before. Since

$$I(S(\tau) : E(\tau)) = \mathscr{D}(\rho_{se}(\tau)||\rho_s(\tau)\otimes\rho_e(\tau)), \tag{1.49}$$

an informational version of the Second Law follows from Klein inequality:

$$\Delta S_s(\tau) + \Delta S_e(\tau) = \mathscr{D}(\rho_{se}(\tau)||\rho_s(\tau)\otimes\rho_e(\tau)) \geq 0. \tag{1.50}$$

This inequality states that, starting with the total knowledge of the two separate systems, we can only end up with a loss of information due to the interaction between the two parts.
Nothing has been said about entropy production, nor of the thermodynamic content: this can be recovered by considering the usual scenario of equilibrium Thermodynamics. Suppose that the initial composite state is made of a system coupled to a heat bath (not necessarily macroscopic) at thermal equilibrium. As we shall see in the next section, these systems are described by the Gibbs state:

$$\rho_e(0) = \frac{e^{-\beta H_e}}{Z_e} := \mathscr{G}_e(\beta). \tag{1.51}$$

The entropy production in this scenario should be

$$< \Sigma(\tau) >= \Delta S_s(\tau) - \beta < Q(\tau) >, \tag{1.52}$$

where $< Q(\tau) >= \mathrm{Tr}_e\left[H_e(\rho_e(\tau) - \mathscr{G}_e(\beta))\right]$. It can be shown that

$$< Q(\tau) >= \mathscr{D}(\rho_e(\tau)||\mathscr{G}_e(\beta)) - \Delta S_s(\tau) + I(S(\tau) : E(\tau)), \tag{1.53}$$

from which we get the elegant formula:

$$\Sigma = \mathscr{D}(\rho_e(\tau)||\mathscr{G}_e(\beta)) + I(S(\tau) : E(\tau)) \geq 0, \tag{1.54}$$

which represents the generalization of the Second Law of Thermodynamics.

The formula explains the increase of entropy as a consequence of two factors. The first term, $\mathscr{D}(\rho_e(\tau)||\mathscr{G}_e(\beta))$, quantifies how much the environment is taken away from equilibrium, while the second term, $I(S(\tau) : E(\tau))$, describes the appearance of correlations between the system and the environment.

1.5 Equilibrium

As in standard Thermodynamics, equilibrium plays a crucial role. One of the foundational questions of quantum Thermodynamics is then: how can we characterize equilibrium states? It is well known that these states have to be of the form of Gibbs: there are different ways to prove it, an elegant one is to make use of Jaynes idea, introduced in [5, 6].

1.5.1 Jaynes principle

The intuition attributed to Jaynes is, in thermodynamic systems, that the knowledge that we have about one particular state is encoded in macroscopic, extensive variables, such as average energy and number of particles. For this

reason, apart from those extensive quantities, we have the minimum possible knowledge about the system: after all, we cannot expect to have information on the dynamics of the single particles involved. On the other hand, the second law of Thermodynamics tells us that for every system S, the amount of entropy either grows or stays the same for any process: it must be, if we are in equilibrium (and thus in a stationary configuration), that the entropy of the system is already the maximum possible, so that it does not grow anymore. This is the logic behind the Jaynes Principle, which is also called "the Maximum Entropy Principle".

Jaynes Principle: the density matrix ρ that best describes the current state of knowledge of a thermodynamic system is the one that maximizes the Von Neumann Entropy $S(\rho)$.

Gibbs States from Jaynes Principle

Now we show that the maximization of entropy leads inequivocally to the Gibbs state. Consider a thermal state ρ, extensive quantities described by the observables $\{A_i\}$, such that $a_i = \mathrm{Tr}[A_i\rho]$, which we consider as conserved quantities $[H, A_i] = 0$. Then we can use the method of Lagrange multipliers to find ρ: we start by defining the Lagrange function

$$\mathscr{L}(\rho) := S(\rho) + \lambda(\mathrm{Tr}[\rho] - 1) + \sum_i \beta_i(\mathrm{Tr}[A_i\rho] - a_i), \tag{1.55}$$

where the second and third terms are zero by definition. To find the maximum, we search for an extremum:

$$\frac{\delta\mathscr{L}(\rho)}{\delta\rho} = 0. \tag{1.56}$$

Taking into account $\rho = \sum_j p_j |j\rangle\langle j|$ with the $\{|j\rangle\}$ set of eigenstates of H, slight variations of ρ means variation of eigenvalues and eigenvectors.
We start from the variations of the eigenvectors. These are described by Stone's Theorem, via unitary operators $U(\theta) = e^{iW\theta}$, where $W = W^\dagger$, θ group parameter. In particular,

$$-i\hbar\delta\rho = [W, \rho]\,\delta\theta. \tag{1.57}$$

This means that, for the variation of eigenstates,

$$\delta\mathscr{L}(\rho) = -\mathrm{Tr}\left[\delta\rho(\log(\rho) + \sum_i \beta_i A_i)\right]. \tag{1.58}$$

Substituting $\delta\rho$ with the above formula, we get:

$$\begin{aligned}\delta\mathscr{L}(\rho) &= -\mathrm{Tr}\left[\frac{i}{\hbar}\delta\theta\,[W,\rho\,](\log(\rho)+\sum_i\beta_i A_i)\right]= \\ &= \mathrm{Tr}\left[\frac{i}{\hbar}\delta\theta W\left[\rho,(\log(\rho)+\sum_i\beta_i A_i)\right]\right]= \\ &= \mathrm{Tr}\left[\frac{i}{\hbar}\delta\theta W\left[\rho,\sum_i\beta_i A_i\right]\right]=0 \\ &\text{iff } \left[\rho,\sum_i\beta_i A_i\right]=0,\end{aligned} \tag{1.59}$$

where we used $\mathrm{Tr}[[A,B]\,C] = \mathrm{Tr}[A[B,C]]$ and $[\rho,\log(\rho)] = 0$. Hence, ρ commutes with $\sum_i \beta_i A_i$. Commutation implies that they share a basis of eigenvectors, thus we can write

$$\sum_i \beta_i A_i = \sum_\alpha A_\alpha \left|\alpha\right\rangle\left\langle\alpha\right|, \tag{1.60}$$

where

$$A_\alpha := \mathrm{Tr}\left[\sum_i \beta_i A_i \left|\alpha\right\rangle\left\langle\alpha\right|\right] \tag{1.61}$$

is the projection of the sum onto the basis vector α. Thus, we can write the Lagrange function as

$$\mathscr{L}(\rho) := -\sum_\alpha \rho_\alpha(\log(\rho_\alpha)-\lambda-A_\alpha), \tag{1.62}$$

which varied with respect to eigenvalues gives:

$$\delta\mathscr{L}(\rho) = -\delta\rho(\log(\rho_\alpha)+1-\lambda-A_\alpha)=0. \tag{1.63}$$

This leads to the solution

$$\rho_\alpha = \frac{e^{-A_\alpha}}{e^{\lambda-1}}, \tag{1.64}$$

where the denominator is fixed by normalization, while the fact that $\rho = \sum_\alpha \rho_\alpha \left|\alpha\right\rangle\left\langle\alpha\right|$ means

$$\rho = \frac{e^{-\sum_i \beta_i A_i}}{e^{\lambda-1}}. \tag{1.65}$$

Defining $Z = \mathrm{Tr}\left[e^{-\sum_i A_i}\right]$, we finally have:

$$\rho = \frac{e^{-\sum_i A_i}}{Z}, \tag{1.66}$$

which is the Gibbs state. The standard form at thermal equilibrium is obtained by inserting as only observable A, the Hamiltonian H, and the associated Lagrange constant β takes the meaning of inverse temperature:

$$\rho = \frac{e^{-\beta H}}{Z(\beta)}. \tag{1.67}$$

1.5.2 Thermalization

While it is clear how to describe states at thermodynamic equilibrium, it is not yet understood how the unitary dynamics of quantum mechanics can lead to such states. In the first place, we define "thermalization" as the process of equilibration toward a thermal state. It is known how to derive thermalization when the system is coupled to an infinite external bath, but the more general derivation for a closed system is still missing. In the classical setting, this is accomplished through the idea of chaos and ergodicity, but the same rules fail when applied to quantum systems.

To explain the problem, consider a quantum system which is initially a pure state $\rho(0) = |\psi(0)\rangle \langle\psi(0)|$, with Hamiltonian $H = \sum_j e_j |e_j\rangle \langle e_j|$. The state in the energy basis becomes

$$|\psi(0)\rangle = \sum_j \langle e_j|\psi(0)\rangle |e_j\rangle = \sum_j c_j |e_j\rangle . \tag{1.68}$$

Its evolution is given by:

$$|\psi(t)\rangle = \mathscr{U} |\psi(0)\rangle = \sum_j c_j e^{-ie_j t/\hbar} |\psi(0)\rangle . \tag{1.69}$$

As we can see, the unitary evolution implies that the system remains a pure state for all $t \geq 0$. Moreover, the state function is multiplied by an oscillating function: there will be moments in which the system reaches its initial configuration! It is clear that the system is strongly dependent on its initial condition: there is no reason to think that it could be represented by a maximally mixed state as the Gibbs state.
Despite this argument, the experiments show that the state does thermalize.
A solution to this apparent paradox is provided by the Eigenstate Thermalization Hypothesis [8]. The key insight is to shift the focus from the global state, which remains pure and unitary, to local observables. Since local subsystems become highly entangled with the rest of the system, their reduced density matrix becomes indistinguishable from a thermal state. This could be formalized by focusing on local observables. In particular, the hypothesis required to

guarantee the emergence of a Gibbsian state is encoded in the structure of the expectation values of these observables: the ETH posits that the diagonal matrix elements of a local operator $\hat{O}$ in the energy eigenbasis vary smoothly with energy. This condition ensures that the individual energy eigenstates already contain the thermal physics of the Gibbs state. Consequently, for any physical state with a well-defined average energy, the long-time expectation value of $\hat{O}$ becomes independent of the specific initial conditions, effectively converging to the thermal prediction:

$$O_{nn} \approx \langle \hat{O} \rangle (e_n), \tag{1.70}$$

where $\langle \hat{O} \rangle$ is the expectation value computed for a Gibbs state. In this framework, thermalization is understood not as the loss of information but as its irreversible spreading into global entanglement, making it inaccessible to any local measurement.

For a complete overview of the hypothesis, see [9].

1.6 The Zeroth and the Third law

1.6.1 The Zeroth Law

Equipped with a well defined characterization of equilibrium states, we can go back to the Zeroth Principle of Thermodynamics and adapt it in the quantum realm. Once one has identified an equilibrium state with the inverse temperature β, the standard statement (Section 1.1) can be reformulated: "Systems in equilibrium with each other have the same temperature". Thus, consider a composite system made of system and environemnt $S + E$ at equilibrium with each other. The total system is described by the thermal state

$$\rho = \frac{e^{-\beta(H_s \otimes \mathbb{1}_e + \mathbb{1}_s \otimes H_e + H_{se})}}{Z(\beta)}. \tag{1.71}$$

If the zeroth principle holds, then the system and environment subsystems must be:

$$\rho_s = \mathrm{Tr}_e[\rho] = \frac{e^{-\beta H_s}}{Z_s(\beta)} \qquad \rho_e = \mathrm{Tr}_s[\rho] = \frac{e^{-\beta H_e}}{Z_e(\beta)} \tag{1.72}$$

But this holds iff $H_{se} = 0$: we can recover the validity of the zeroth law of Thermodynamics only in the weak coupling regime, i.e. when $H_{se} << H_s, H_e$. For strong coupling regimes, we have a non trivial situation in which two systems can be in equilibrium with a third system, but not within each other!

1.6.2 The Third Law

In the form of Nernst unattainably principle, the third law of Thermodynamics states that it is impossible to cool a system to its ground state without diverging resources.
Despite being experimentally accepted for a long time, a general derivation in the framework of standard Thermodynamics is still subject of ongoing research. It is with the advent of quantum mechanics and the rederivation of quantum Thermodynamics that the principle acquired new light. From a quantum perspective, cooling a system to zero temperature means the complete purification of a mixed state. It has been shown that this task cannot be accomplished without diverging resources [10], where resources can be time, energy, or control complexity [11].

This is the principle that mostly influenced our work: since perfect cooling cannot be accomplished, the only positive outcome will be to have upper bound on the minimum temperature reached (see Section 2.3).

1.7 Maximal Work Extraction

In this section, we deal with one of the oldest problems of Thermodynamics, which is that of finding the maximal amount of work that can be extracted from a system S by means of an external source of work acting ciclically in a thermally isolated process. Its finite quantum version takes the name "ergotropy" - according to [12] - and was first addressed in [13] under the name of "adiabatic availability". In light of the definition of work given for closed system, we already know how the problem should be posed. Consider a system S, which is closed and initially described by the time independent Hamiltonian H, undergoing an additional time dependent term $V(t)$ that acts as the external source of work, such that $H(t) = H + V(t)$, with $V(0) = V(t_f) = 0$. Since the system is closed, the extracted work is given by

$$W = \Delta U = \mathrm{Tr}[H\rho(0)] - \mathrm{Tr}\big[H\rho(t_f)\big],$$

where $\rho(0)$ is the initial density matrix, and $\rho(t_f)$ is given by the unitary evolution $\mathscr{U}$: $\rho(t_f) = \mathscr{U}(t_f)\rho(0)\mathscr{U}^\dagger(t_f)$ induced by the hamiltonian $H(t) = H + V(t)$. Once $\rho(0)$ is fixed, the maximal extractable work corresponds to solving the maximization problem

$$\max_{\mathscr{U}}\Big\{\mathrm{Tr}\big[H(\rho(0) - \mathscr{U}\rho(0)\mathscr{U}^\dagger)\big]\Big\} =: \mathscr{E}(\rho), \tag{1.73}$$

which is the mathematical definition of ergotropy. Since the initial energy is fixed, we can only act on the second term: the extracted work is maximal when the final energy is at minimum. Calling $E_f = \mathrm{Tr}\left[H\mathscr{U}\rho(0)\mathscr{U}^\dagger\right]$ the final energy and $E_f^\star$ the minimal accessible final energy, we want to find $\mathscr{U}$ s.t. $E_f^\star = \mathrm{Tr}\left[H\mathscr{U}\rho(0)\mathscr{U}^\dagger\right]$.

To find the minimum, we proceed in the style of classical mechanics variational problems: we consider small variations of the variables contained in E_f and search for an extremum point. This translates into considering small displacements of the unitary evolution $\delta\mathscr{U}$, which we parameterize through $\delta\mathscr{U} = X\mathscr{U}$, where X is an infinitesimal and anti-Hermitian operator. Indeed, we find $\delta E_f = \delta(\mathrm{Tr}\left[H\mathscr{U}\rho(0)\mathscr{U}^\dagger\right]) = \mathrm{Tr}\left[H\delta\mathscr{U}\rho(0)\mathscr{U}^\dagger + H\mathscr{U}\rho(0)(\delta\mathscr{U})^\dagger\right]$, since H and $\rho(0)$ are considered fixed. This leads to

$$\delta E_f = \mathrm{Tr}\left[X\left[\mathscr{U}\rho(0)\mathscr{U}^\dagger, H\right]\right].$$

The extremum condition $\delta E_f = 0$ requires for the final state $\mathscr{U}\rho(0)\mathscr{U}^\dagger = \rho(t)$ to be commuting with H: $\rho(t)$ has the same eigenvalues of $\rho(0)$ and shares eigenvectors with H. Writing the spectral decomposition of $\rho(0)$ and H

$$\rho(0) = \sum_i p_i \left|i\right\rangle\left\langle i\right| \qquad\qquad H = \sum_j e_j \left|e_j\right\rangle\left\langle e_j\right|, \tag{1.74}$$

we can build the final state with minimum energy:

$$\rho(t) = \sum_k p_k \left|e_k\right\rangle\left\langle e_k\right| \qquad\qquad p_{k+1} \geq p_k,\ e_{k+1} \leq e_k. \tag{1.75}$$

The correct final state is obtained by ordering the eigenvalues in such a way that low energy eigenstates of H have a higher probability. This guarantees that, when taking the trace to compute the average final energy, one gets $E_f = \sum_k p_k e_k$, which coincides with the minimum final energy $E_f^\star$.

Chapter 2

Quantum Thermodynamics for Quantum Computing

In recent years, there has been an increasing interest in the field of quantum computation and information. This area of research has the promising virtue of performing particular tasks, like simulation of physical systems, optimization or drug discovery, exponentially faster than classical computation [14, 15]. Furthermore, quantum mechanics provides the foundation for inherently secure communication through quantum cryptography protocols.

For this reason, a number of new companies have been founded with the goal of building a reliable quantum computer in the near future.

If, on one side, making computation "quantum" guarantees undeniable advantages, on the other it requires managing microscopic systems and their delicate properties. Indeed, to run a standard quantum algorithm we need to perform unitary operations on a closed quantum system: this can be done faithfully by isolating the working qubits from the environment. This, in general, is impossible: in real-world, no isolated quantum system actually exists (apart from the universe itself, perhaps), and one should deal with errors occurring from the interaction with the outside world. To reduce those errors, quantum processors must be cooled at extremely low temperatures: it turned out that the theory of quantum Thermodynamics can provide a lot of tools to accomplish this task.
In this chapter, we explore one such tool: the initialization of qubits in a pure state through algorithmic cooling. This process consists in reducing the temperature of a selected qubit by running an algorithm that redistributes the entropy with the effect of increasing the temperature of ancillary qubits.

The chapter is structured as follows. In the first part - Section 2.1 - we briefly introduce the theory of quantum computation, where we introduce some of the definitions that will be used over the course of the chapter. In the subsequent sections, we shift the attention to the problem of initialization. Starting from the theory of algorithmic cooling in Section 2.2 we then introduce two algorithms that have been recently published in Sections 2.3,2.4.

2.1 Quantum Computation

Over the course of the twentieth century, some of the most sophisticated theories in modern science came to life. While quantum mechanics revolutionized our understanding of reality at the microscopic scale, Turing's theory of computation provided the conceptual framework for computational machines, enabling the solution of complex mathematical problems through a "calculator".

Initially, the latter was far from being a physical theory: its foundations were deeply embedded in mathematical logic and Boolean algebra. However, as the century progressed, the scientific community moved toward a more physical interpretation of information - and vice versa - as epitomized by Wheeler's famous "it from bit" doctrine, which suggests that information may play a crucial role in the fundamental laws of physics. The first formal bridge between these two branches was built by Landauer [16], who demonstrated that the erasure of one bit of information is necessarily associated with a minimum heat dissipation of $k_B T \log 2$.

The history of quantum computation properly began in the early 1980s, when Richard Feynman published his seminal article "Simulating Physics with Computers" [14]. In it, he demonstrated the inherent inefficiency of classical computation in simulating quantum systems and suggested that a proper computational model should itself be quantum, thus proposing the conceptual foundation for quantum computers.

In this section, we explore the consequences of this insight by translating the fundamental building blocks of classical computation into the language of quantum mechanics.

2.1.1 Quantum Bits, Quantum Circuits

In classical computation and information theory, the structure of the theory is centered upon the transmission and manipulation of information. To quantify such information, the concept of the bit is introduced as the fundamental unit.

A bit represents the most basic form of data: a binary quantity that can exist in one of two mutually exclusive states, 0 or 1, corresponding to "true/false" or "yes/no" statements.

The Qubit

When extending this definition to a quantum mechanical framework, the situation changes fundamentally. While the orthonormal basis states $|0\rangle$ and $|1\rangle$ can represent classical bits, the linearity of quantum theory implies that any normalized linear combination of these states is also a valid state of the system:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \tag{2.1}$$

where $\alpha, \beta \in \mathbb{C}$ are complex probability amplitudes subject to the normalization condition $|\alpha|^2 + |\beta|^2 = 1$.

This principle of superposition makes the qubit a far more mathematically rich object than its classical counterpart. While a classical bit is restricted to the poles of a discrete set, a qubit can exist in a continuum of states.

A more intuitive way to visualize the state of a single qubit is through the Bloch sphere representation. Since the state vector $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ must be normalized ($|\alpha|^2 + |\beta|^2 = 1$), and since an overall global phase $e^{i\gamma}$ does not result in observable physical differences, we can re-parameterize the qubit using two real-valued angles, θ and ϕ:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{2.2}$$

where $0 \leq \theta \leq \pi$ defines the polar angle and $0 \leq \phi < 2\pi$ defines the azimuthal angle (see Figure 2.1).

Quantum Gates

The word "computation" refers to the transformation and processing of information. This is accomplished, in classical theory, with the application of logic gates on the string of bits under exam. In the same way, in quantum computation, we perform computation by applying quantum gates to the qubit.

Mathematically, as required by the postulates of quantum theory for a closed system, a quantum gate acting on a single qubit is represented by a unitary operator $\mathcal{U}$ acting on the state space. The unitarity condition, $\mathcal{U}^\dagger\mathcal{U} = I$, ensures that the normalization of the state vector is preserved, reflecting the reversible nature of quantum evolution.

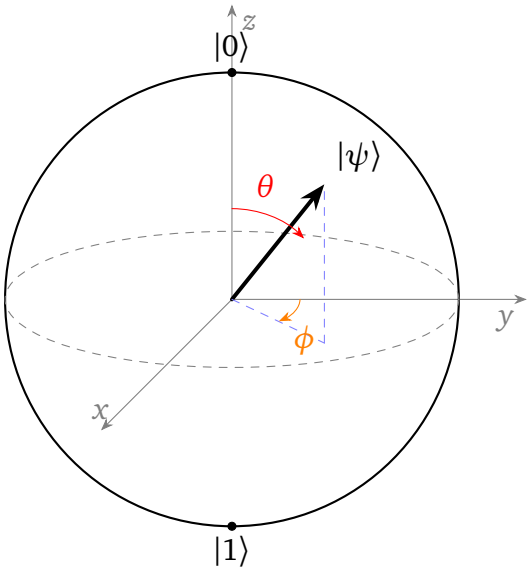

Figure 2.1: Representation of a qubit state $|\psi\rangle$ on the Bloch Sphere.

The most fundamental single-qubit gates are the Pauli matrices, which in the computational basis are defined as:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.3}$$

The X gate acts as a quantum NOT, flipping $|0\rangle$ to $|1\rangle$ and vice versa. The Z gate is a phase-flip operator, essential for creating relative phases. Another crucial operator is the Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{2.4}$$

which acts on the computational basis as:

$$\begin{aligned} H|0\rangle &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \equiv |+\rangle, \\ H|1\rangle &= \frac{|0\rangle - |1\rangle}{\sqrt{2}} \equiv |-\rangle. \end{aligned} \tag{2.5}$$

It is worth introducing a two-qubit logic gate: the Controlled Not (CNOT).

In a two-qubit system, the state space is the tensor product of the individual Hilbert spaces, $\mathscr{H}_1 \otimes \mathscr{H}_2$, spanned by the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

The CNOT gate involves a control qubit and a target qubit. Its action is to flip the state of the target qubit if and only if the control qubit is in the state $|1\rangle$. Mathematically, if we denote the control as the first qubit and the target as the second, the operation is defined as:

$$\begin{aligned} \text{CNOT}|00\rangle &= |00\rangle \\ \text{CNOT}|01\rangle &= |01\rangle \\ \text{CNOT}|10\rangle &= |11\rangle \\ \text{CNOT}|11\rangle &= |10\rangle \end{aligned} \tag{2.6}$$

After having introduced single qubit gates and the CNOT, we could think of doing the same procedure for 2 qubits, then 3,.. . Clearly, we soon realize that there is an infinite number of operations that one can perform on a particular string of qubits (if the string number is not fixed). For this reason, a crucial question in computer science regards the possibility of building increasingly complex logic operations as composition of finite elementary gates: this is the concept of "universality".
In classical computation, this is solved by the universality of the NAND gate: is there a solution for the quantum version of the problem?

Quantum Universality

A first answer to the question posed above is given by the following result:

Theorem 2.1.1. *Single qubit gates $R(\theta, \phi)$ and CNOT are universal for quantum computation*

This provides a first general answer. However, the set is uncountably infinite, as it requires to be able to perform rotations $R(\theta, \phi)$ by an arbitrary angle θ and ϕ in the Bloch sphere.
From a practical perspective, it is more relevant to look for a discrete set of gates. In this way, once it is possible to reproduce faithfully this discrete set of operations in an experiment, one would be able to perform an arbitrary operation on qubits.
It turns out that a discrete set of gates is indeed sufficient to approximate any general unitary operation to arbitrary precision:

Theorem 2.1.2 (Solovay-Kitaev Theorem)**.** *A discrete set of gates is universal for quantum computation in the sense that any unitary operation can be approximated to within an error $\epsilon > 0$ using a sequence of $O(poly(\log(1/\epsilon)))$ gates from the set.*

For example, a universal discrete set of gates is $\{H, R_{\pi/4}, \text{CNOT}\}$, where

$$R_\phi := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}.$$

2.1.2 Quantum Algorithms

The existence of a universal set of gates implies that any desired transformation of a quantum system can be decomposed into a sequence of elementary operations, forming what is known as a quantum algorithm. From a physical perspective, an algorithm is essentially a controlled unitary evolution $\mathscr{U}$ designed to map an initial state ρ to a final state $\rho' = \mathscr{U}\rho\mathscr{U}^\dagger$, such that specific information is processed or concentrated.

As an example of a quantum algorithm, we now expose the Quantum Fourier Transform, which will become crucial later in order to solve problems encountered in our work.

Example: The Quantum Fourier Transform

The Quantum Fourier Transform (QFT) is the quantum analogue of the discrete Fourier transform, and it constitutes the core component of many powerful quantum algorithms, including phase estimation, Shor's factoring algorithm, and hidden subgroup problems. As discussed in Nielsen and Chuang [15], the QFT performs a linear transformation on quantum states that is equivalent to the classical DFT, but with the advantage of exponential speedup in terms of the number of gates required.

Formally, the discrete Fourier transform maps a vector of complex numbers $(x_0, \ldots, x_{N-1})$ to another vector $(y_0, \ldots, y_{N-1})$ according to the formula:

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j e^{2\pi i jk/N} \tag{2.7}$$

The Quantum Fourier Transform is defined similarly as a linear operator $\mathscr{F}$ acting on the orthonormal basis states $\{|0\rangle, \ldots, |N-1\rangle\}$, where $N = 2^n$ and n is the number of qubits. The action of the QFT on a basis state $|j\rangle$ is given by:

$$\mathscr{F}|j\rangle := \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i jk/N} |k\rangle \tag{2.8}$$

Equivalently, for an arbitrary state $|\psi\rangle = \sum_j x_j |j\rangle$, the transformation yields $\sum_k y_k |k\rangle$, where the coefficients y_k are the discrete Fourier transform of the amplitudes x_j.

An important property for the circuital implementation of the QFT is its ability to be expressed in a product form. Using the binary representation of the integer $j = j_1 j_2 \dots j_n$ (where $j = \sum_{l=1}^{n} j_l 2^{n-l}$), the output state can be factored as:

$$|j_1 \dots j_n\rangle \rightarrow \frac{(|0\rangle + e^{2\pi i 0.j_n}|1\rangle) \otimes (|0\rangle + e^{2\pi i 0.j_{n-1}j_n}|1\rangle) \otimes \cdots \otimes (|0\rangle + e^{2\pi i 0.j_1 j_2 \dots j_n}|1\rangle)}{2^{n/2}} \tag{2.9}$$

where we use the binary fraction notation $0.j_l j_{l+1} \dots j_n = \sum_{m=l}^{n} j_m 2^{-(m-l+1)}$.

Another interesting property of the QFT can be shown in the picture of density matrices. Suppose that a quantum state is initially described by a diagonal density matrix ρ, with diagonal elements λ_i, which, for generality, are all different from each other. What does the action of a QFT yield for such a state?

Representing the state as

$$\rho = \sum_{j=1}^{N} \lambda_j |j\rangle \langle j|, \tag{2.10}$$

with $|j\rangle$ for $j = 1, .., N$ form the basis of eigenvectors, and N dimension of the Hilbert space, we have:

$$\begin{aligned}
\rho' = \mathscr{F}\rho\mathscr{F}^\dagger = \sum_{j=1}^{N} \lambda_j \mathscr{F}|j\rangle\langle j|\mathscr{F}^\dagger = \\
= \sum_{j=1}^{N} \lambda_j \left(\frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i jk/N}|k\rangle\right)\left(\frac{1}{\sqrt{N}} \sum_{l=0}^{N-1} e^{-2\pi i jl/N}\langle l|\right) = \\
= \sum_{j=1}^{N} \frac{\lambda_j}{N} \left(\sum_{k,l=0}^{N-1} e^{(k-l)2\pi i jk/N}|k\rangle\langle l|\right).
\end{aligned} \tag{2.11}$$

We can now compute the diagonal element of the final state ρ':

$$\begin{aligned}
\langle m|\rho'|m\rangle = \langle m| \sum_{j=1}^{N} \frac{\lambda_j}{N} \left(\sum_{k,l=0}^{N-1} e^{(k-l)2\pi i jk/N}|k\rangle\langle l|\right)|m\rangle = \\
= \sum_{j=1}^{N} \frac{\lambda_j}{N} \left(\sum_{k,l=0}^{N-1} e^{(k-l)2\pi i jk/N}\langle m|k\rangle\langle l|m\rangle\right) = \\
= \sum_{j=1}^{N} \frac{\lambda_j}{N}.
\end{aligned} \tag{2.12}$$

This shows a remarkable property of the QFT: applying the QFT to a diagonal state leads to a final state that is not diagonal, but whose diagonal is made of N identical elements that are equal to the mean of the eigenvalues $\sum_j \lambda_j/N$.

2.1.3 Requirements for Quantum Computation

Thus far, we spoke about quantum computation and quantum computer by mentioning abstract entities as "qubit" and "unitary gate", but what does it really take to build physical objects that are able to perform such operations?

One should start with a system that is described properly as a two-level quantum system in order to describe such a "quantum bit". For example, a $1/2$ spin particle would be able to properly describe a qubit through the identification of the spin state $|\downarrow\rangle$ with $|0\rangle$ and $|\uparrow\rangle$ with $|1\rangle$. On the other hand, such a system should be initialized through some process to its logical state $|0\rangle$, which translates into an initial pure state:

$$\rho = |0\rangle \langle 0| . \tag{2.13}$$

This is required for computational reasons: one needs to know precisely with which state the computation starts to ensure the reliability of the algorithm. Moreover, we should also be able to do this operation on N such systems, in order to have more computational power

$$\rho = |0\rangle \langle 0|^{\otimes N} . \tag{2.14}$$

This must be done in such a way that it works globally in the same way it does locally, i.e. the system must be scalable. Quantum operations are then implemented by controlling a suitable Hamiltonian H, often via external drives or electromagnetic pulses. According to the Schrödinger equation, this induces a unitary evolution

$$\mathscr{U}(t_{eff}, 0) = \mathscr{T} \exp\left(-\frac{i}{\hbar} \int_0^{t_{eff}} H(t')dt'\right), \tag{2.15}$$

where the operator $\mathscr{T}$ represents the time ordering. By precisely tuning the interaction time t_{eff} and the Hamiltonian parameters, one can faithfully implement any desired unitary $\mathscr{U}$. As discussed in Section 2.1, the ability to perform a universal set of discrete gates (discrete set of single-qubit rotations and CNOT) is sufficient to approximate any transformation: once we build an experimental setup that guarantees the ability to perform such set of operations, we can realize arbitrary unitaries. Furthermore, the qubits must remain

isolated from the environment to avoid decoherence - the loss of quantum information due to unwanted interactions. The characteristic decoherence time T_d must be significantly longer than the time required to perform a gate operation. Last but not least, we need to be able to perform "quantum efficiently" measurements, i.e. if a state is $\rho = p\,|0\rangle\langle 0| + (1-p)\,|1\rangle\langle 1|$ we must measure $|0\rangle$ with probability p.

All of these arguments have been elegantly summarized by DiVincenzo [17] through a set of 5 requirements that an hypothetical quantum computer should fulfill:

- a scalable physical system with well defined qubits,
- the ability to initialize qubits in the logical state 00..0,
- qubit's long decoherence time, at least much longer than the gate operation duration,
- the ability to perform a universal set of quantum gates,
- the ability to measure specific qubits.

Once we satisfy all of these requirements, we can claim to have built a quantum computer.

2.2 Algorithmic Cooling

As mentioned in Section 2.1, one of the requirements to perform quantum computation is the ability to initialize qubits in the logical state 00...00, i.e. to have qubits in the pure state $|00...00\rangle$ (under the assumption that qubits are diagonalized in the same basis). Unfortunately, it is physically impossible to reach that condition through cooling, and the reason lies in the third principle of Thermodynamics: initializing qubits physically means that they have to be cooled, and the state $|00..00\rangle$ corresponds to the ground state. This is not the end of the game, though: it is not strictly necessary to have a pure state: it is enough to have a quantum state which is almost pure, i.e. pure with an error δ. For example, consider a single qubit quantum computer, with initial state

$$\rho_Q = (1-\delta)\,|0\rangle\langle 0| + \delta\,|1\rangle\langle 1|,$$

this is not pure, but if we take δ to be small enough, the chances of getting $|1\rangle$ after a measurement will be negligible. The initialization of quantum bits translates into the task of minimizing δ: this can be done by cooling, be it physical or algorithmic.

For physical cooling, we refer to those techniques that are used to cool qubits or, in general, the quantum computer via physical methods. This particular task is accomplished in different ways based on the particular type of quantum computer we are using: for example, for superconducting qubits, diluition refrigerators are used, or laser cooling for particular systems of trapped ions.
Algorithmic cooling, on the other hand, refers to the method of cooling qubits via (quantum) algorithm: in principle, we add redundancy to our system in the form of ancillary qubits, and we use this to extract entropy from selected qubits, with the effect of puryfing them at expenses of the ancillas. We must say that in the laboratory these two techniques are not separated: usually quantum computers are physically cooled at the beginning and then undergo algorithmic cooling to increase the fidelity of the initial quantum state.
There are two ways of performing algorithmic cooling: closed system algorithmic cooling and open system algorithmic cooling.

2.2.1 Closed system

The first idea for cooling single qubits was suggested by Shulman and Vazirani [18], according to developments in quantum algorithms, why not use an algorithm to cool qubits?

In their work, they consider a closed quantum system of N qubits, acting as a reversible heat engine which absorbs energy to perform a separation of hot and cold regions inside the system. The idea is then to discard the hot regions and ending the cycle with the cold region as output, represented by M cold qubits (see Figure 2.2).

The framework was thought to be used for NMR quantum computers - molecules where qubits are represented by the nuclear spins embedded in the molecule. For these systems, it is convenient to use the polarization ϵ to quantify the population:

$$\epsilon := n(e_0) - n(e_1), \tag{2.16}$$

where $n(e)$ is the occupation number at energy e and e_0 and e_1 are ground state energy and excited state energy of the spin, respectively. Thus, consider the single qubit density matrix, written as a function of the polarization ϵ:

$$\rho_\epsilon = \frac{1+\epsilon}{2} |0\rangle \langle 0| + \frac{1-\epsilon}{2} |1\rangle \langle 1|, \tag{2.17}$$

the total initial state is considered to be the mixed state given by

$$\rho = \bigotimes_{i=1}^{N} \rho_\epsilon^{(i)}. \tag{2.18}$$

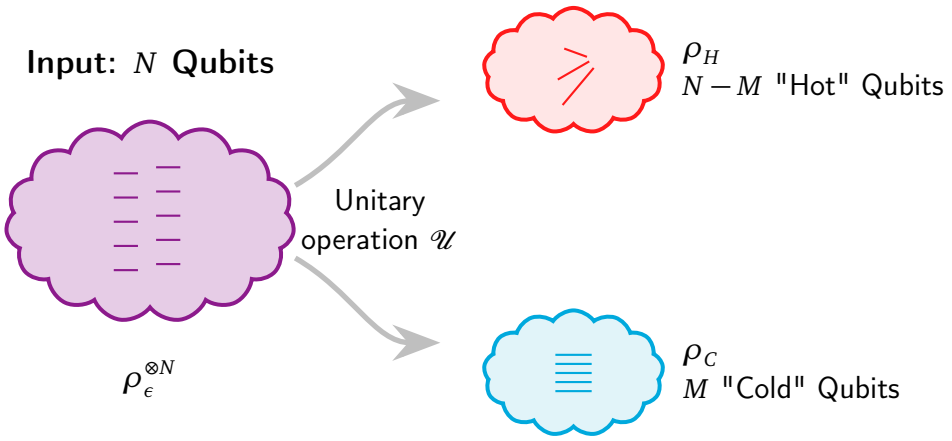

Figure 2.2: Scenario of closed system based algorithmic cooling: a set of N qubits described by the thermal state with polarization ϵ is manipulated by a quantum circuit to perform separation between a cold region and a hot region. The cold region will be the output initialized qubits to be used in the quantum computer.

The algorithm corresponds to implementing the unitary operation $\mathscr{U}$ that performs the separation: the final state is

$$\rho' = \mathscr{U}\rho\mathscr{U}^\dagger = \mathscr{U}\left(\bigotimes_{i=1}^{N}\rho_\epsilon^{(i)}\right)\mathscr{U}^\dagger. \tag{2.19}$$

The regions are described by the partial trace:

$$\begin{aligned}\rho_H &= \mathrm{Tr}_C\left[\rho'\right],\\ \rho_C &= \mathrm{Tr}_H\left[\rho'\right],\end{aligned} \tag{2.20}$$

where the subscripts H and C stand for "hot" and "cold". The dimensions of the state space of the regions depend on the number of qubits M that we are able to cool. For this prototype, the authors showed that it is possible to reach a final configuration where M qubits have polarization of order of unity (purified qubits), where

$$M = N\left[\frac{1+\epsilon}{2}\log(1+\epsilon)+\frac{1-\epsilon}{2}\log(1-\epsilon)-o(1)\right], \tag{2.21}$$

with ϵ polarization of the initial N qubits [18].

Unfortunately, in real liquid state NMR quantum computers the initial entropy reducing preparation is weak: polarization results to be very small. On the

other hand, the unitary dynamics imposed by the closed system is naturally constrained to obey the Shannon bound: we have a limit on the entropy we can extract from selected qubits since the total entropy must be conserved. For a bipartite system $T+A$, which is initially a separable state $\rho = \rho_T \otimes \rho_A$, and defining ρ_i' as final states of the subsystem i, this is given by:

$$S(\rho_T') \geq S(\rho_T) + S(\rho_A) - S(\rho_A'). \tag{2.22}$$

2.2.2 Heat Bath Algorithmic Cooling

To overcome the problems found in closed systems, open systems dynamics-based algorithms have been introduced [19]. The general idea is to introduce an interaction with an external environment, which enables the transfer of entropy from the target qubits into an effectively infinite reservoir, thereby overcoming the Shannon bound.

A nice example to get an idea of the method was given in [20].
Here we explain the most simple prototype of Heat Bath algorithmic cooling, represented in Figure 2.3.
Let

$$\rho = \bigotimes_{i=1}^{N} \rho_\epsilon^{(i)} \tag{2.23}$$

be the density matrix of the initial system, composed of N ϵ-polarized qubits. Qubits are dinguished by their role: we call "target qubits" the first M qubits, which are the one that are to be cooled, and we call "ancilla" (or "reset") the qubits that extract entropy from the target.
The algorithm is structured in two steps:

- entropy compression,
- interaction with the environment.

In the "entropy compression" phase, a closed system algorithm is performed. The system evolves through a unitary operation: this extracts entropy from the M target qubits and adds it to the $N-M$ ancillary qubits. At the end of the first phase we reach the final configuration explained for closed system dynamics: a hot region made of reset qubits described by ρ_A separated from a cold region ρ_T of target qubits. Here we used subscripts to identify the type of qubit: "A" for the ancillas and "T" for the targets.
At this point, the open system dynamics comes into play: we let the ancilla qubits interact with a cold external heat reservoir at inverse temperature β_e. This extracts entropy from the reset qubits until they reach thermal equilibrium

with the reservoir at temperature β_e:

$$\rho_A'' = \bigotimes_{i=1}^{N-M} \mathcal{G}(\beta_e), \tag{2.24}$$

where $\mathcal{G}(\beta)$ are the Gibbs state at inverse temperature β. At the end of the two steps, we end up with the state:

$$\rho_{HB} = \rho_T' \otimes \rho_A''. \tag{2.25}$$

This state has smaller entropy than the initial one, ρ: the open system dynamics enables us to reach configurations that in closed systems are prohibited by entropy conservation. Note that we can potentially run this algorithm all the times we need: at each step, we compress the entropy into the $N-M$ qubits and then discard it into the heat bath.

In the last decades, new proposals for candidates to perform quantum computation have been published. While in the early 2000 the interest was mostly for NMR quantum computation, now new promising frameworks have been introduced, such as superconducting qubits and high fidelity trapped ions. These frameworks present promising properties, starting from their ability in reaching extremely cold temperatures through physical cooling. This recently pushed scientific interest in re-evaluate techniques that were dismissed in the development of NMR quantum computation, such as closed system algorithmic cooling.

2.3 Dynamic Cooling

Recently, an interesting proposal on a cooling algorithm based on closed system dynamics was given in [21], we refer to it as "Dynamic Cooling". Considering N identical qubits in thermal equilibrium at some temperature T, we can cool the first one by finding an optimal unitary operation $\mathcal{U}$ on the global system such that the first qubit is as cold as possible (see Figure 2.4).

The questions we want to address are: what is the optimal $\mathcal{U}$? How much can we cool?

2.3.1 Optimal Unitaries

Given the description above, the initial system is described by the global state

$$\rho = \bigotimes_{k=1}^{N} \frac{e^{-\beta H_k}}{Z_k(\beta)}, \tag{2.26}$$

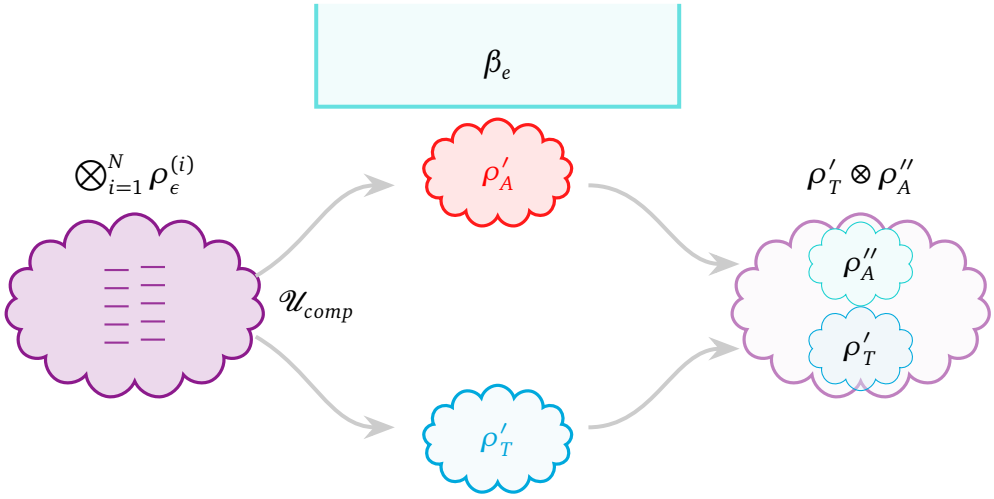

Figure 2.3: Representation the algorithm presented in our example. An initial state made of N ϵ-polarized qubits represented as the purple cloud, undergoes a unitary operation $\mathcal{U}_{comp}$, which compresses entropy inside $N-M$ reset qubits. This process cools the target system, which is represented by the light blue cloud ρ'_T. Meanwhile, reset qubits, which are represented as the red cloud (the hot region) ρ'_A, are placed in contact with the heat reservoir at temperature β_e. The region evolves through a non unitary evolution until it reaches thermodynamic equilibrium at temperature β_e, reaching the state ρ''_A: in this process it discards the entropy into the reservoir. The final state is given by the lower entropy bipartite state $\rho'_T \otimes \rho''_A$, represented by the ligther cloud on the right.

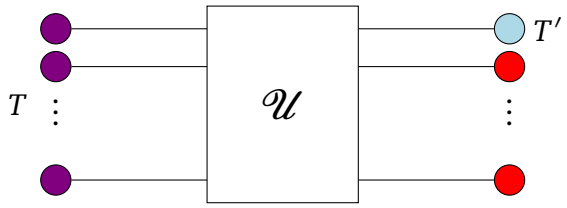

Figure 2.4: Schematic representation of Dynamic Cooling: N initial qubits undergo the unitary global evolution $\mathcal{U}$, whose goal is to cool the first qubit as much as possible, at the expenses of heating up the other $N-1$ qubits.

where the single qubit Hamiltonian is $H_k = \frac{\hbar\omega}{2}\sigma_z^{(k)}$ acts only on the k-th qubit, $\beta = \frac{1}{k_B T}$ is the inverse temperature and k_B the Boltzmann constant. The partition function $Z_k(\beta)$ of the k-th qubit becomes $Z_k(\beta) = e^{-\beta\hbar\omega/2} + e^{\beta\hbar\omega/2} = 2\cosh(\beta\hbar\omega/2)$. After the action of the global unitary $\mathscr{U}$, the state becomes $\rho' = \mathscr{U}\rho\mathscr{U}^\dagger$, and the target state ρ_1' is its partial trace with respect to the ancillas:

$$\rho_1' = \mathrm{Tr}_A\left[\rho'\right] = \frac{e^{-\beta' H_1}}{Z_1(\beta')}, \tag{2.27}$$

where the qubit acquires inverse temperature β' and the subscript A refers to the ancillary system. The final state of the ancillas, composed of the $N-1$ qubits, in general describes a system of non-identical qubits with a local higher temperature compared to β.
Asking for the final target qubit to be the coldest is equivalent to asking for it to be at minimal energy. By introducing the final target qubit Hamiltonian $K_1 := H_1 \otimes \mathbf{1} \otimes ... \otimes \mathbf{1}$ and the target qubit energy $u := \mathrm{Tr}[K_1\rho]$ we can define the optimal unitary operator as the one that minimizes u' (the final energy of the target qubit):

$$u' = \min_U \left\{\mathrm{Tr}\left[K_1 \mathscr{U}\rho\mathscr{U}^\dagger\right]\right\}. \tag{2.28}$$

This should look familiar: it is the same minimization problem that occurs in the definition of ergotropy (see Section 1.7), i.e. the maximal extractable work from a quantum system. Indeed, the definition of ergotropy in this framework is

$$\mathscr{E}(\rho) := \max_{\mathscr{U}} \left\{\mathrm{Tr}\left[K_1\rho\right] - \mathrm{Tr}\left[K_1\mathscr{U}\rho\mathscr{U}^\dagger\right]\right\}, \tag{2.29}$$

where we can isolate the second term, which is the only one that contains $\mathscr{U}$, and get Equation 2.28. As argued in Section 1.7, ergotropy has a well known solution $\mathscr{U}$ when $[\rho, K_1] = 0$: it is the unitary operation that permutes the eigenvalues of ρ, p_i, in such a way that the highest ones are associated to the lower energy eigenstates of K_1. Thus, the final state is described as

$$\rho' = \sum_i p_i \left|e_i\right\rangle \left\langle e_i\right|, \tag{2.30}$$

where $e_i \leq e_{i+1}$ are the energy eigenstates of K_1 and $p_i \geq p_{i+1}$ are the reordered eigenvalues of ρ.

2.3.2 Cooling Temperature

Once we know the optimal $\mathscr{U}$, it is easy to compute the final temperature of the target qubit. In fact, we can isolate the target qubit final state by tracing

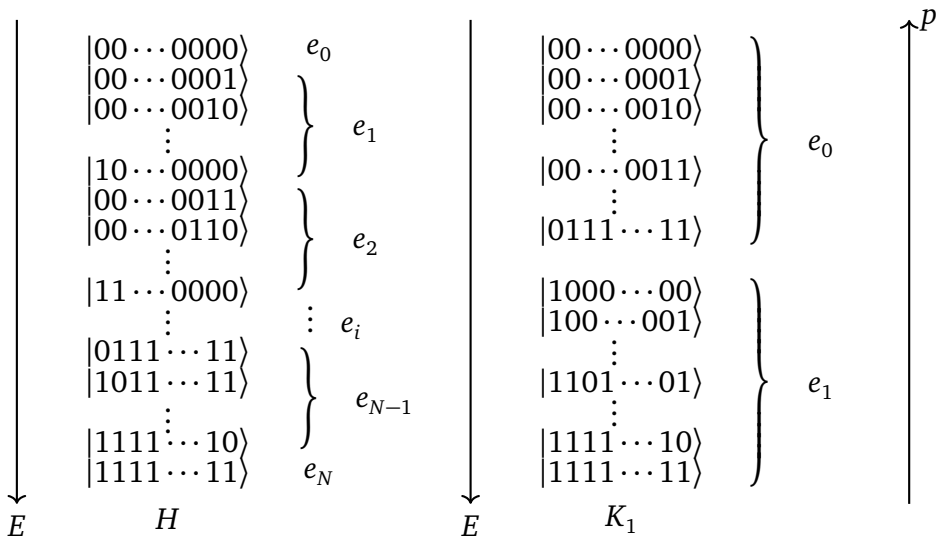

Figure 2.5: Scheme that summarizes the spectral evolution. Initially ρ is the thermal state under Hamiltonian H. Its eigenvalues are related to eigenvalues of H through the Gibbs distribution: states with total energy e_i have probability $p = e^{-\beta e_i}/Z$, and this is greater as e_i is smaller. On the other side eigenvalues of K_1 are just two: e_0 and e_1, where the first is associated to eigenstates that have a "zero" as first digit and the second is associated to those that have "one". Thus we order the probabilities in such a way that e_0 eigenstates are in 1-1 correspondence with the first 2^{N-1} probability elements $e^{-\beta e_i}/Z$, counted with their multiplicity. Note that we have freedom in choosing which of the 2^{N-1} highest eigenvalues must be mapped to a particular eigenstate of e_0.

out the ancillas:

$$\rho_1' = \mathrm{Tr}_A\left[\rho'\right] = P_0' \left|0\right\rangle \left\langle 0\right| + P_1' \left|1\right\rangle \left\langle 1\right|. \tag{2.31}$$

Since there are only two eigenvalues e_0, e_1 of K_1 with degeneracy 2^{N-1}, the probabilities are divided into 2 sets: the highest 2^{N-1} are associated with eigenstates of e_0, while the others with eigenstates of e_1. This means that P_0' is just the sum of the highest 2^{N-1} eigenvalues, while P_1' is the sum of the lowest half, as shown in Figure 2.5.

For this reason, we can explicitly compute P_1' and study the final cooling temperature as a function of the initial one. Taking into account that the initial

eigenvalues are also degenerate with binomial degeneracy, we get

$$P_1'(P_1,N) = \sum_{0\le k<N/2} \binom{N}{k}(1-P_1)^k P_1^{N-k} + \left(2^{N-1} - \sum_{0\le k<N/2}\binom{N}{k}\right)(1-P_1)^{N/2}P_1^{N/2}. \tag{2.32}$$

In particular, the second term of the formula considers the terms needed from the central degenerate state to complete the sum. For this reason, this will be zero for N odd, since there is no central degenerate state, and different from zero for N even. Indeed, we can rewrite Equation 2.32 by explicitly separating the two scenarios:

$$P_1'(P_1,N) = \sum_{0\le k<N/2} \binom{N}{k}(1-P_1)^k P_1^{N-k} \quad \text{for } N \text{ odd}, \tag{2.33}$$

$$P_1'(P_1,N) = \sum_{0\le k<N/2} \binom{N}{k}(1-P_1)^k P_1^{N-k} + \frac{1}{2}\binom{N}{N/2}(1-P_1)^{N/2}P_1^{N/2} \quad \text{for } N \text{ even}. \tag{2.34}$$

An interesting observation is that if we start with an odd number of qubits, adding an additional one will not decrease the target qubit temperature:

$$P_1'(P_1, 2s-1) = P_1'(P_1, 2s), \tag{2.35}$$

as proved in [21]. This means also that, starting from $N = 1$, the addition of a 1 single qubit will not lead to cooling: to cool a qubit, a number of at least 2 ancillas is needed. Another meaningful observation can be made. Looking at the plot shown in Figure 2.6 one can notice that, for increasing N, P_1' tends to zero. Asymptotically

$$\lim_{N\to\infty} P_1'(P_1,N) = 0, \tag{2.36}$$

which holds $\forall\ P_1 < \frac{1}{2}$. This is the third principle of Thermodynamics: to cool down the target qubit to zero temperature we would need infinite resources, which in this case are ancillary qubits.

Once we have an explicit formula for P_1', we can find the final temperature T'. In fact, we only need to take the inverse of $P_1' = 1/(e^{\beta'\hbar\omega}+1)$, which gives

$$\frac{k_B T'}{\hbar\omega} = \frac{1}{\log((1/P_1'(P_1,N))-1)}. \tag{2.37}$$

Moreover, one can find the function $T'(T)$ by explicitly writing P_1' as a function of P_1, and this as a function of T, leading to a highly non-trivial formula.

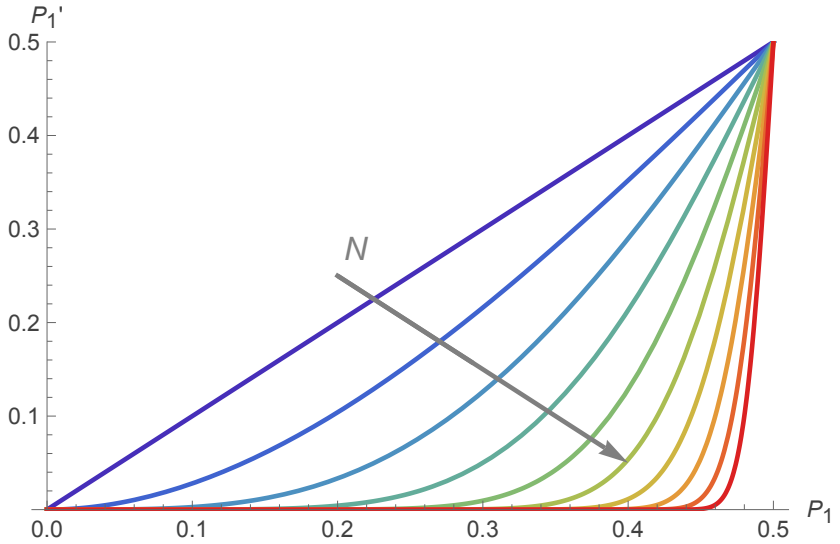

Figure 2.6: Plot of $P_1'(P_1,N)$ for $N=2^j$ for $j\in[1,10]$. For $N=2$ the function is a straight line: $P_1'=P_1$, according to the fact that 3 qubits are necessary to have cooling. For higher N, P_1' becomes smaller.

2.3.3 Estimates for the Temperature

To quantify how much we can cool a single qubit, it is more convenient to look at asymptotic regimes, i.e. to look at cooling temperature for high initial T and low T.

High temperature regime

In the high temperature regime $P_1'=1/(1+e^{\beta'\hbar\omega})\to 1/2$ for $T\to\infty$. Thus, we approximate P_1' by expanding it around $P_1=1/2$:

$$P_1'(P_1,N)=P_1'(1/2,N)+\left.\frac{\partial P_1'(P_1,N)}{\partial P_1}\right|_{P_1=1/2}(P_1-1/2)+O((P_1-1/2)^2).$$

To obtain general results despite the parity of N, we use the fact that $P_1'(P_1,2s-1)=P_1'(P_1,2s)$ and write all terms as functions of $N=2s-1$. The term of zero order is, by trivial substitution, $P_1'(1/2,N)=1/2$. Meanwhile, the first order term is

$$C_s:=\left.\frac{\partial P_1'(P_1,2s-1)}{\partial P_1}\right|_{P_1=1/2}=\frac{1}{2^{2s-2}}\sum_{0\le k<N/2}(2s-2k-1)\binom{2s-1}{k}. \tag{2.38}$$

This turns out to be equal to $C_s=2^{2-2s}s\binom{2s-1}{s}$. At the same time, we find low-β Taylor expansions relations for the excited state populations, yielding to

$P_1 = 1/2 - \beta\hbar\omega/4$. Taking the high temperature limit on both initial and final states, we get

$$\beta'\hbar\omega = C_s\beta\hbar\omega \tag{2.39}$$

If we also assume the limit for large N, we can make use of Stirling approximation for C_s: indeed we have $N! \simeq \sqrt{2\pi N}(N/e)^N$, which gives $C_s \simeq (2/\sqrt{\pi})\sqrt{s}$.

Putting all of this together, we find a high tempertaure, high N estimate for the cooling temperature of the target qubit:

$$T' \simeq \sqrt{\frac{\pi}{2}}\frac{T}{\sqrt{N}} \tag{2.40}$$

Low temperature regime

For small T, $P_1 = 1/(1+e^{\beta\hbar\omega}) \to 0$, we can Taylor expand P_1' around $P_1 = 0$:

$$P_1'(P_1, N) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k P_1'(P_1, N)}{\partial P_1^k}\bigg|_{P_1=0} P_1^k. \tag{2.41}$$

For every $k < s$, the Taylor coefficients are zero. The first non-zero term is the one at order s, and reads

$$a_s := \frac{\partial^s P_1'(P_1, N)}{\partial P_1^s}\bigg|_{P_1=0} = \binom{2s-1}{s}. \tag{2.42}$$

Thus, the lowest order expansion of P_1' is:

$$P_1'(P_1, 2s-1) = a_s P_1^s + O(P_1^{s+1}) \tag{2.43}$$

Again, we can obtain a more meaningful estimate for the temperature. We consider the excited state population $P_1 = 1/(1+e^{\beta\hbar\omega})$, which, at first order for $1/\beta \to 0$, becomes $P_1 = e^{-\beta\hbar\omega}$. Assuming low initial temperature guarantees also low final temperature (since this is always smaller): we can substitute the first order approximation for P_1 and P_1' into Equation 2.43 to obtain

$$\beta'\hbar\omega = \beta\hbar\omega s - \log(a_s). \tag{2.44}$$

By taking, again, the high β limit, the log term can be neglected, leading to the final formula

$$T' \simeq \frac{1}{s}T = \frac{2}{N}T. \tag{2.45}$$

This formula shows a much better scaling compared to the high temperature one, meaning that dynamic cooling is more suitable for cooling qubits that start from a low temperature.

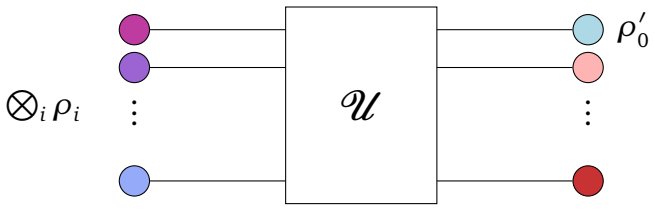

Figure 2.7: Typical scenario of Dynamic Cooling with non identical initial qubits. According to the situation described, we associate the target qubit - the first one at the top - to highest initial temperature and machine qubits with temperature that step by step smaller: the last machine qubit - the one at the bottom - is the colder. Undergoing the unitary $\mathscr{U}$, the target qubit is cooled at the expenses of the machine qubits, which increase their temperature.

2.4 Dynamic Cooling with non-identical machine qubits

Suppose now that the initial qubits are not identical, can we still say something? This is the scenario studied in [22], where the focus shifts to finding general properties of the cooling process.
Consider the situation represented in Figure 2.7, where N non-identical qubits undergo a unitary operation $\mathscr{U}$ that cools one of them. What can we say about the temperature of this qubit?

2.4.1 3 qubits example

The analysis starts with a simple example that already exhibits some of the features that will be encountered in the general case. Consider a system composed of three qubits, each one with a different energy gap:

$$\begin{aligned}\rho_s &= \frac{|0\rangle\langle 0| + e^{-\omega}|1\rangle\langle 1|}{Z_s},\\ \rho_{m_1} &= \frac{|0\rangle\langle 0| + e^{-\gamma_1}|1\rangle\langle 1|}{Z_{m_1}},\\ \rho_{m_2} &= \frac{|0\rangle\langle 0| + e^{-\gamma_2}|1\rangle\langle 1|}{Z_{m_2}}.\end{aligned} \tag{2.46}$$

The first density matrix describes the "system qubit" (or the target), which is the qubit that has to be cooled. The second and third density matrices describe

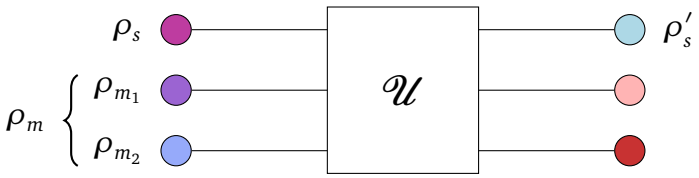

Figure 2.8: Adaptation of Figure 2.7 to the case with 3 intial qubits - 2 machine qubits. By ρ_s we denote the density matrix of the target qubit, while ρ_{m_i} is the state of the "i"-th machine qubit, with $\rho_m = \rho_{m_1} \otimes \rho_{m_2}$. At the same time, ρ_s' represent the cooled target qubit at the end of the algorithm.

ancilla qubits, which we call "machine qubits", as they are part of the machine that will extract heat from the target. Energy gaps are ordered such that the target qubit is the hottest, while the machine ones are colder: $\omega \leq \gamma_1 \leq \gamma_2$. For a graphical representation of the framework, see Figure 2.8. The total system is the tensor product of the single qubits:

$$\rho = \rho_s \otimes \rho_{m_1} \otimes \rho_{m_2} = \sum_{i \in \{0,1\}^3} \frac{e^{-\mathrm{i}\Lambda} |i\rangle \langle i|}{Z_s Z_m}, \tag{2.47}$$

where $\mathbf{i} = \{i_0, i_1, i_2\}$ is the vector of the string $i = i_0 i_1 i_2$, $|i_0 i_1 i_2\rangle := |i_0\rangle \otimes |i_1\rangle \otimes |i_2\rangle$, $\Lambda := \{\omega, \gamma_1, \gamma_2\}$ and $Z_m = Z_{m_1} Z_{m_2}$ is the machine partition function and Z_s that of the target system. The initial excited state population of the target qubit is given by

$$\langle 1| \rho_s |1\rangle = \frac{e^{-\omega}}{Z_s} = \langle 1| \mathrm{Tr}_m [\rho] |1\rangle = \sum_{i_M \in \{0,1\}^2} \frac{e^{-\omega - i_M \Gamma}}{Z_s Z_m}, \tag{2.48}$$

where $\Gamma := \{\gamma_1, \gamma_2\}$. Coincidentally, the ground state population is:

$$\langle 0| \rho_s |0\rangle = \frac{1}{Z_s} = \langle 0| \mathrm{Tr}_m [\rho] |0\rangle = \sum_{i_M \in \{0,1\}^2} \frac{e^{-i_M \Gamma}}{Z_s Z_m}. \tag{2.49}$$

Is it possible, throught a unitary operation $\mathscr{U}$, to increase the ground state population of the target? Can we beat the temperature of the coldest machine qubit?

By now, it must be clear that the only unitary operation that minimizes energy is the one that permutes eigenvalues: the idea is to map eigenstates corresponding to the target ground state to highest eigenvalues, in complete analogy to what we did before. This is what is done in Figure 2.9: to maximize the population of the ground state of the target qubit, we must

- swap eigenvalues $e^{-\omega}/Z$ and $e^{-\gamma_1 - \gamma_2}/Z$,

- swap eigenvalues $e^{-(\omega+\gamma_1)}/Z$ and $e^{-\gamma_2}/Z$ iff $\omega < \gamma_2 - \gamma_1$.

Now, consider the two cases separately.

Case 1: $\omega \geq \gamma_2 - \gamma_1$

In this case, only one permutation occurs. The final target qubit ground state population becomes:

$$P_0 = \frac{1 + e^{-\omega} + e^{-\gamma_2} + e^{-\gamma_1}}{Z_s Z_m}, \tag{2.50}$$

which can be shown to be greater than $\langle 0| \rho_{m_2} |0\rangle$, which is the ground state population of the coldest of the initial machine qubits. This means that, by choosing 3 qubits with gaps $\omega \leq \gamma_1 \leq \gamma_2$ such that $\omega \geq \gamma_2 - \gamma_1$, we can cool one qubit further than the coldest qubit!

Case 2: $\omega < \gamma_2 - \gamma_1$

In the other case, the final target qubit ground population reads:

$$P_0 = \frac{1 + e^{-\omega} + e^{-(\omega+\gamma_1)} + e^{-\gamma_1}}{Z_s Z_m} = \frac{(1 + e^{-\omega})(1 + e^{-\gamma_1})}{Z_s Z_m} = \frac{1}{Z_{m_2}}. \tag{2.51}$$

Basically, the cooling unitary operation is just a SWAP with the coldest machine qubit! This means, on the other hand, that one machine qubit is not needed and that the algorithm is not cooling overall: we start with two qubits that have some temperature β_i, and we end up with the same temperatures, just swapped between the two qubits. This is the situation that one would like to avoid in the implementation of the initialization.

2.4.2 General Case: Fundamental inequalities for permutations

In the general case, we refer again to Figure 2.7. N non-identical qubits undergo a unitary operation that cools the first one, the "system" qubit. According to the example with $N = 3$ qubits, we consider an increasing gap structure: the system qubit has an energy gap ω, while machine qubits have a gap γ_i such that $\omega \leq \gamma_1 \leq ... \leq \gamma_{N-1}$. The state of the system qubit is

$$\rho_s = \frac{|0\rangle\langle 0| + e^{-\omega} |1\rangle\langle 1|}{Z_s}, \tag{2.52}$$

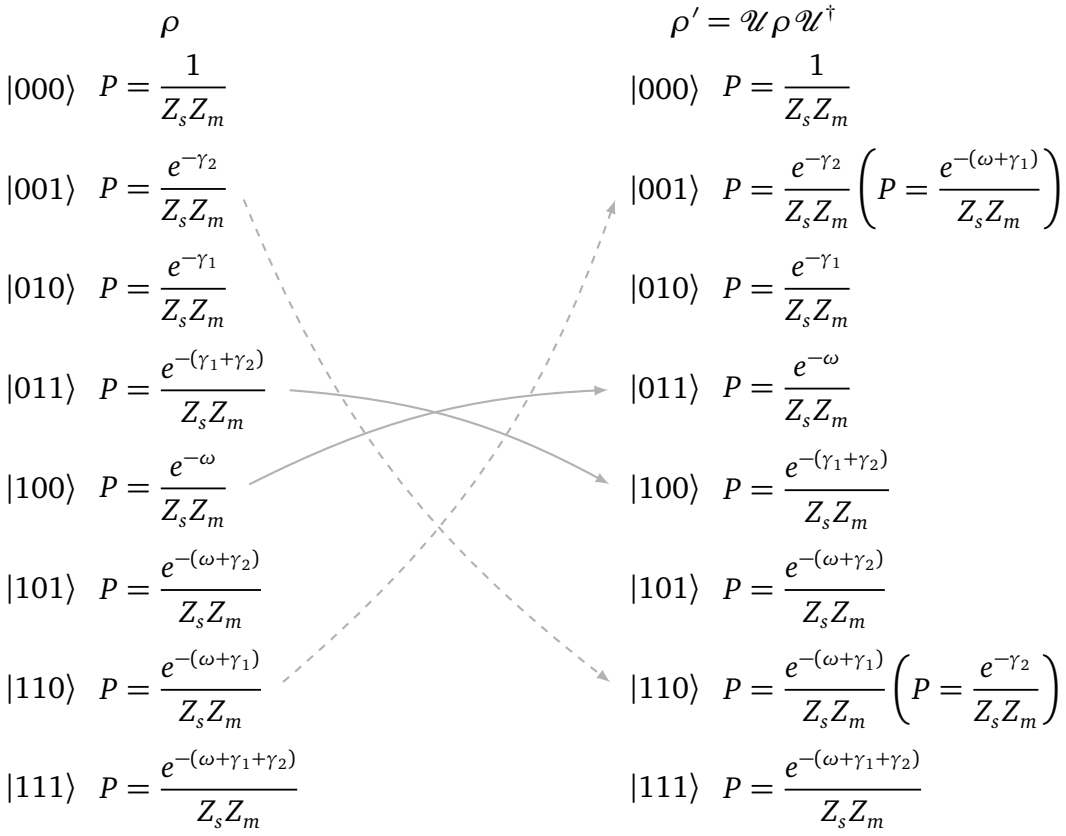

Figure 2.9: Here eigenvectors and eigenvalues of the density matrix are represented. In the left side the spectral structure is referred to the initial state ρ, while in the right side it is referred to ρ', which is the state after the permutations to maximize cooling of the target qubit. Taking under exam the smallest eigenvalue associated with the target qubit ground eigenstate $|011\rangle$, we can see how this is always smaller than the highest eigenvalue associated with excited state target qubit $|100\rangle$: the permutation $|100\rangle \leftrightarrow |011\rangle$ must always be done since $e^{-\omega} > e^{-\gamma_1+\gamma_2}$. The second smallest eigenvalue is the one associated with $|001\rangle$, and the second highest for excited target state is $|110\rangle$. By comparison it turns out that the permutation $|001\rangle \leftrightarrow |110\rangle$ must be done iff $e^{-(\omega+\gamma_1)} > e^{-\gamma_2}$, which is true iff $\omega < \gamma_2 - \gamma_1$ (for this reason, arrows are dotted, and the potential permutation has been located in the parentheses).

while that of the i-th machine qubit is

$$\rho_s = \frac{|0\rangle\langle 0| + e^{-\gamma_i}|1\rangle\langle 1|}{Z_{m_i}}. \tag{2.53}$$

Thus, the initial state of the total composite system is:

$$\rho = \rho_s \otimes \rho_m = \rho_s \bigotimes_{i=1}^{N-1} \rho_{m_i} = \sum_{\substack{i_s\in\{0,1\} \\ j_m\in\{0,1\}^{N-1}}} \frac{e^{-(i_s\omega + j_m\Gamma)}|i_s j_m\rangle\langle i_s j_m|}{Z_s Z_m}, \tag{2.54}$$

where we define the $N-1$ dimensional vector $\Gamma := (\gamma_1, ..., \gamma_{N-1})$. According to the example with $N = 3$, a permutation $|0_s j_m\rangle \leftrightarrow |1_s j'_m\rangle$ must be performed if and only if

$$\frac{e^{-j_m\Gamma}}{Z_s Z_m} < \frac{e^{-(\omega + j'_m\Gamma)}}{Z_s Z_m}. \tag{2.55}$$

This inequality translates into the following condition:

$$\omega < (j_m - j'_m)\cdot\Gamma. \tag{2.56}$$

Adopting the same method used in the example, which consists in comparing the lowest eigenvalue of the eigenstates $|0_s i_m\rangle$ with the highest eigenvalue of the eigenstates $|1_s i_m\rangle$, then the second lowest with the second highest, and so on, it can be shown that the condition becomes:

$$\omega < (j_m - j_m \oplus 1)\cdot\Gamma, \tag{2.57}$$

where $\oplus$ denotes the bitwise addition modulo 2. Explicitly,

$$(j_m \oplus 1)\cdot\Gamma = \sum_{i=1}^{N-1}(j_m \oplus 1)_i\gamma_i = \sum_{i=1}^{N-1}\gamma_i - \sum_{i=1}^{N-1}(j_m)_i\gamma_i = E_g - \omega - j_m\cdot\Gamma, \tag{2.58}$$

where $E_g := \omega + \sum_{i=1}^{N-1}\gamma_i$ is the sum of the total energy gaps of the initial qubits. Using E_g, the condition becomes extremely compact:

$$\frac{E_g}{2} < j_m\cdot\Gamma, \tag{2.59}$$

with clear meaning: "given the string $|0_s j_m\rangle$, switch its eigenvalue with that of $|1_s j_m \oplus 1\rangle$ if and only if Equation 2.59 holds".

Quantifying Cooling

Given a specific structure of the energy gaps of the initial qubits (ω, Γ), we can compute the final ground state population of the target qubit P_0. Indeed, this is identical to the initial ground state population P_0, apart from those terms that have been switched during the cooling protocol. Defining the set of strings that have to be permuted,

$$\mathbb{S} := \{i_m \in \{0,1\}^{N-1} : E_g < 2i_m \cdot \Gamma\}, \tag{2.60}$$

we obtain for the excited state population:

$$P_0' = \sum_{i_m \in \{0,1\}^{N-1} \setminus \mathbb{S}} \frac{e^{-i_m \Gamma}}{Z_s Z_m} + \sum_{i_m \in \mathbb{S}} \frac{e^{-(\omega + (i_m \oplus 1)\Gamma)}}{Z_s Z_m}. \tag{2.61}$$

The variation of the population of the ground state, $\Delta P_0 := P_0' - P_0$, is given by:

$$\Delta P_0 = \sum_{i_m \in \mathbb{S}} \frac{e^{-(\omega + (i_m \oplus 1)\Gamma)} - e^{-i_m \Gamma}}{Z_s Z_m}. \tag{2.62}$$

Substituting, as before, $(i_m \oplus 1)\Gamma = E_g - \omega - i_m \Gamma$, we obtain:

$$\Delta P_0 = \sum_{i_m \in \mathbb{S}} \frac{e^{-E_g} e^{i_m \Gamma} - e^{-i_m \Gamma}}{Z_s Z_m}. \tag{2.63}$$

As claimed in the beginning, once we know the particular structure of energy gaps, we can compute this quantity.

2.4.3 Application: Identical qubits

Now we can close the circle by considering a scenario in which the machine's energy gaps are all equal to that of the target qubit, and proving that this leads to Equation 2.32. Let $\Gamma := (\omega, ..., \omega)$ be the $N-1$ dimensional vector made of the energy gap structure of the machine qubits, and ω the energy gap of the target qubit. Then $E_g = \omega + (N-1)\omega = N\omega$ and for a string $i_m \in \{0,1\}^{N-1}$ we have $i_m \Gamma = w(i_m)\omega$, with $w(i_m)$ Hamming weight of the string i_m. This implies, for the permutation set $\mathbb{S}$, that:

$$\mathbb{S} := \{i_m \in \{0,1\}^{N-1} : N\omega < 2w(i_m)\omega\} \equiv \{i_m \in \{0,1\}^{N-1} : w(i_m) > N/2\}. \tag{2.64}$$

Now, the set $\mathbb{S}$ is that of strings with Hamming weight greater than $N/2$, where we assume N even for simplicity. Moreover, once this set is known, it is easy to compute the excited state probability of the final target qubit:

$$P_1' = \sum_{i_m \in \mathbb{S}} \frac{e^{-i_m \Gamma}}{Z_s Z_m} + \sum_{i_m \in \{0,1\}^{N-1} \setminus \mathbb{S}} \frac{e^{-(\omega + (i_m \oplus 1)\Gamma)}}{Z_s Z_m}. \tag{2.65}$$

Since $i_m \Gamma = w(i_m)\omega$ and by defining $P_0 := 1/Z$ and $P_1 := e^{-\omega}/Z$ where $Z = Z_s = Z_{m_i}$, the excited state probability becomes

$$P_1' = \sum_{i_m \in \mathbb{S}} \frac{e^{w(i_m)\omega}}{Z_s Z_m} + \sum_{i_m \in \{0,1\}^{N-1} \setminus \mathbb{S}} \frac{e^{-\omega} e^{-w(i_m \oplus 1)\omega}}{Z_s Z_m}. \tag{2.66}$$

The sum can be conveniently written in terms of the Hamming weights w, since both probabilities and the set $\mathbb{S}$ are written in terms of them:

$$P_1' = \sum_{\substack{i_m \in \{0,1\}^{N-1} \\ w(i_m) > N/2}} \frac{e^{w(i_m)\omega}}{Z_s Z_m} + \sum_{\substack{i_m \in \{0,1\}^{N-1} \\ w(i_m) \leq N/2}} \frac{e^{-\omega} e^{-w(i_m \oplus 1)\omega}}{Z_s Z_m}, \tag{2.67}$$

and since there are $\binom{N-1}{w}$ strings with Hamming weight "w":

$$P_1' = \sum_{w=N/2+1}^{N-1} \binom{N-1}{w} P_0^{N-w} P_1^{w} + \sum_{w=0}^{N/2} \binom{N-1}{w} P_0^{w} P_1^{N-w}. \tag{2.68}$$

For the symmetry of the binomial $\binom{N-1}{w} = \binom{N-1}{N-1-w}$, we can change the interval of the sum and merge the two:

$$\begin{aligned} P_1' &= \sum_{w=0}^{N/2-2} \binom{N-1}{w} P_0^{w+1} P_1^{N-1-w} + \sum_{w=0}^{N/2} \binom{N-1}{w} P_0^{w} P_1^{N-w} \\ &= \sum_{w=1}^{N/2-1} \binom{N-1}{w-1} P_0^{w} P_1^{N-w} + P_1^N + \sum_{w=1}^{N/2} \binom{N-1}{w} P_0^{w} P_1^{N-w} \\ &= \sum_{w=1}^{N/2-1} \left[\binom{N-1}{w-1} + \binom{N-1}{w} \right] P_0^{w} P_1^{N-w} + \binom{N-1}{N/2} P_0^{N/2} P_1^{N/2} + P_1^N. \end{aligned} \tag{2.69}$$

The term inside the square brackets is equal to $\binom{N-1}{w}$ by Pascal's identity and $\binom{N-1}{N/2} = \frac{1}{2}\binom{N}{N/2}$. The equation can be rewritten in the familiar form:

$$P_1' = \sum_{w=0}^{N/2-1} P_0^{w} P_1^{N-w} + \frac{1}{2}\binom{N}{N/2} P_0^{N/2} P_1^{N/2}, \tag{2.70}$$

which is identical to Equation 2.32 for N even. This provides the formal equivalence between the two approaches adopted.

Chapter 3

Single shot cooling of multiple qubits

In the previous chapter, we discussed ways to cool a single qubit given ancillary resources. In reality, to see a quantum advantage one needs a lot more computational power than a single qubit. This means that we need the initialization in a pure state of a higher number of elements, which translates to the task of cooling multiple qubits. This can be obtained in two ways: the first is to run in parallel M cooling algorithms, which will give as output M cold qubits, while the second is to perform a specific algorithm that would be able to cool down multiple qubits with a single unitary operation. While, for the former, the bounds introduced in Chapter 2 still hold, for the latter we need in the first place to build the correct unitary operation and then to quantify how much this is able to cool the targets.

3.1 Unitaries for identical qubits

The first scenario that we take into consideration is in analogy with the one of dynamic cooling: N identical qubits at thermal equilibrium at temperature T undergo a unitary operation $\mathscr{U}$ acting on the total space, such that, as output, $M < N$ target qubits are cooled at the expenses of the ancillary $N - M$ ones (see Figure 3.1).

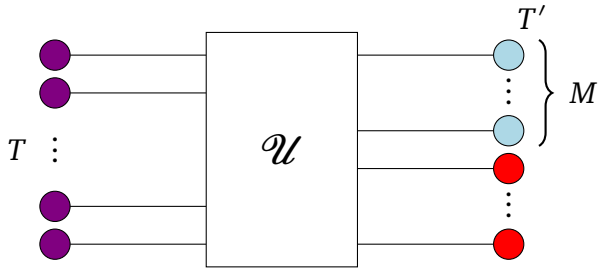

Figure 3.1: N thermal qubits (purple) at temperature T undergo a unitary operation $\mathscr{U}$ that cools M of them (blue) to temperature T', at expenses of the others (red). Note that, even though ancillary qubits are drawn as red, they are not, in general, at the same temperature.

3.1.1 Optimal Unitaries

The initial state framework is completely identical to the one of dynamic cooling. The density matrix reads

$$\rho = \bigotimes_{i=1}^{N} \frac{e^{-\beta H_i}}{Z_i(\beta)}, \tag{3.1}$$

where $H_i = \hbar\omega\sigma_z^i/2$ is the Hamiltonian of single qubit, $\beta = 1/K_B T$ the inverse temperature, K_B is the Boltzmann costant and $Z_i(\beta) = Tr(e^{-\beta H_i}) = 2\cosh(\beta\hbar\omega/2)$ is the partition function.

The goal of the cooling algorithm is to cool the target qubits such that all the targets end up with the same temperature T'. This requirement imposes a strong constraint on the dynamics of the system:

- the operator $\mathscr{U}$ must minimize the energy of the M target qubits (cooling requirement),
- the operator $\mathscr{U}$ must lead to a final state composed of locally identical qubits (unique temperature requirement).

Under these conditions, the final state of the target qubits would be

$$\rho'_T := \mathrm{Tr}_A\left[\rho'\right] = \bigotimes_{i=1}^{M} \frac{e^{-\beta' H_i}}{Z_i(\beta')} + \rho'_{corr}, \tag{3.2}$$

where the subscript "A" in the partial trace means that we are tracing out the ancillary system from the total state ρ', while β' refers to the cooled temperature T' and ρ'_{corr} is a traceless operator that contains possible correlations.

The goal is to find the minimal cooling temperature T' that the target qubits can reach.

Cooling requirement

Asking for the lowest temperature for the final M qubits is equivalent to requiring minimal energy. With this purpose we introduce the Hamiltonian that describes the energy of the target qubits

$$\begin{aligned} K_M =& H_1 \otimes \mathbb{1} \otimes ... \otimes \mathbb{1} + \mathbb{1} \otimes H_2 \otimes \mathbb{1} \otimes ... \otimes \mathbb{1} + \\ &+ ... + \mathbb{1} \otimes ... \otimes \mathbb{1} \otimes H_M \otimes \mathbb{1} \otimes ... \otimes \mathbb{1}, \end{aligned} \tag{3.3}$$

and the problem becomes:
What is the operator $\mathscr{U}$ that minimizes the final energy of the target qubits?
Defining u'_M as the final energy of the target qubit, we have $u'_M = Tr(K_M \mathscr{U} \rho \mathscr{U}^\dagger)$. The operator $\mathscr{U}$ is the one that solves the minimization problem

$$u'_M = \min_{\mathscr{U}} \{\mathrm{Tr}(K_M \mathscr{U} \rho \mathscr{U}^\dagger)\}, \tag{3.4}$$

which, again, coincides with the ergotropy. Following step by step the argument exposed in Section 2.3, we obtain as unitary operator the one that permutes eigenvalues of ρ by mapping the highest to lowest K_M energy eigenvectors. The final state is

$$\rho' = \sum_i p_i \left|e_i\right\rangle \left\langle e_i\right|, \tag{3.5}$$

where now e_i represent the eigenvalues of K_M, ordered such that $e_{i+1} \geq e_i$ and $p_{i+1} \leq p_i$ are the initial eigenvalues of ρ.

Unique Temperature requirement

The Hamiltonian K_M is highly degenerate: this leaves some freedom in the choice of the best $\mathscr{U}$ to fulfil also the equal temperature condition. The problem becomes to translate this requirement at the level of the density matrix. We start by identifying states that have the same temperature: given $j \in [1, M]$ target qubits have the same temperature iff $\rho'_j = P'_0 \left|0\right\rangle \left\langle 0\right| + P'_1 \left|1\right\rangle \left\langle 1\right|$, where P'_0 and P'_1 are independent of j. On the other hand, the target qubits subspaces are found by partial tracing out ancillary qubits and the other targets apart from the one under exam:

$$\rho'_j = \mathrm{Tr}_A \mathrm{Tr}_{T\setminus\{j\}} \left[\rho'\right], \tag{3.6}$$

where the subscript $T \setminus \{j\}$ represents the system composed of all target qubits except the j-th.

At this point, we make two crucial observations. The first is given by the following theorem:

Theorem 3.1.1. *Let ρ be a diagonal density matrix in some basis B, $\mathcal{U}$ a unitary matrix that permutes eigenstates.*
Then $\rho' = \mathcal{U}\rho\mathcal{U}^\dagger$ is a diagonal density matrix in the same basis B.

Proof. Since $\mathcal{U}$ permutes eigenstates: $U|\epsilon_i\rangle = |\epsilon_{\sigma(i)}\rangle$
Meanwhile, ρ is diagonal in the energy basis:

$$\rho = \sum_i p_i |\epsilon_i\rangle \langle\epsilon_i| .$$

Thus

$$\rho' = \mathcal{U}\rho\mathcal{U}^\dagger = \sum_i p_i \mathcal{U}|\epsilon_i\rangle \langle\epsilon_i| \mathcal{U}^\dagger = \sum_i p_i |\epsilon_{\sigma(i)}\rangle \langle\epsilon_{\sigma(i)}|,$$

which is still diagonal. □

Moreover, we can write the final state in a block diagonal form, where we separate the target system from the ancillary system:

$$\rho' = \sum_{i_T \in \{0,1\}^M} |i_T\rangle \langle i_T| \otimes \rho_{A_{i_T}}, \tag{3.7}$$

where $\rho_{A_{i_T}}$ represents the density matrix of the ancillary system corresponding to the configuration i_T for the first M digits. In matrix form:

$$\rho' = \begin{bmatrix} \rho_{A_{0\ldots0}} & & & \\ & \rho_{A_{0..01}} & & \\ & & \ddots & \\ & & & \rho_{A_{1\ldots1}} \end{bmatrix}. \tag{3.8}$$

Note that, to represent ρ' in this way, we ordered eigenstates with K_M, which for $M > 2$ is no longer coincident with the computational basis.

Now, all is set to search for a condition for the unique temperature. We start from $M = 1$ and, step by step, generalize to arbitrary M.
According to Equation 3.7, for $M = 1$, the final state can be decomposed between the target system and the auxiliary system as

$$\rho' = |0\rangle\langle 0| \otimes \rho_{A_0} + |1\rangle\langle 1| \otimes \rho_{A_1}. \tag{3.9}$$

In matrix form:

$$\rho' = \begin{bmatrix} \rho_{A_0} & \mathbf{0} \\ \mathbf{0} & \rho_{A_1} \end{bmatrix}. \tag{3.10}$$

We can obtain the target qubit density matrix from ρ' by tracing out the ancillary system:

$$\rho'_1 = \mathrm{Tr}_A\left[\rho'\right] = \mathrm{Tr}\left[\rho_{A_0}\right]|0\rangle\langle 0| + \mathrm{Tr}\left[\rho_{A_1}\right]|1\rangle\langle 1|. \tag{3.11}$$

This is the result found in Section 2.3: $P'_1 = \mathrm{Tr}\left[\rho_{A_1}\right]$ is the sum of the smallest probabilities up to half of the states.

For $M = 2$ the situation changes: the target system has dimension 4 and in the computational basis the final density matrix is represented by the mixed state:

$$\begin{aligned} \rho' = |00\rangle\langle 00| \otimes \rho_{A_{00}} + |01\rangle\langle 01| \otimes \rho_{A_{01}} + \\ + |10\rangle\langle 10| \otimes \rho_{A_{10}} + |11\rangle\langle 11| \otimes \rho_{A_{11}}. \end{aligned} \tag{3.12}$$

We can compute local states by taking the partial trace over the other system: $\rho'_1 = \mathrm{Tr}_2\left[\rho'_T\right]$ and $\rho'_2 = \mathrm{Tr}_1\left[\rho'_T\right]$ where $\rho'_T = \mathrm{Tr}_A[\rho']$. One gets

$$\rho'_1 = \left(\mathrm{Tr}\left[\rho_{A_{00}}\right] + \mathrm{Tr}\left[\rho_{A_{01}}\right]\right)|0\rangle\langle 0| + \left(\mathrm{Tr}\left[\rho_{A_{10}}\right] + \mathrm{Tr}\left[\rho_{A_{11}}\right]\right)|1\rangle\langle 1|, \tag{3.13}$$

$$\rho'_2 = \left(\mathrm{Tr}\left[\rho_{A_{00}}\right] + \mathrm{Tr}\left[\rho_{A_{10}}\right]\right)|0\rangle\langle 0| + \left(\mathrm{Tr}\left[\rho_{A_{01}}\right] + \mathrm{Tr}\left[\rho_{A_{11}}\right]\right)|1\rangle\langle 1|. \tag{3.14}$$

Clearly,

$$\rho'_1 = \rho'_2 \qquad \text{iff} \qquad \mathrm{Tr}\left[\rho_{A_{01}}\right] = \mathrm{Tr}\left[\rho_{A_{10}}\right]. \tag{3.15}$$

Thus, if the eigenvalues can be ordered in a way such that this condition holds, then the two target qubits will have the same temperature.
We can follow this line of reasoning and provide a condition for identical states for generic M. Similarly to what we did for $M = 2$, we represent the final density matrix according to Equation 3.7. Tracing out the ancillay system, we can compute the density matrix of the target subsystem:

$$\rho'_T = \sum_{i_T \in \{0,1\}^M} \mathrm{Tr}\left[\rho_{A_{i_T}}\right] |i_T\rangle \langle i_T| . \tag{3.16}$$

Now it is possible to compute single state density matrices. Since we are searching for a condition that guarantees local equality, it is enough to compute the excited state population of a single qubit. For the k-th qubit:

$$\langle 1|\rho'_k|1\rangle = \sum_{\substack{i_T \in \{0,1\}^M \\ (i_T)_k = 1}} \mathrm{Tr}\left[\rho_{A_{i_T}}\right] = \sum_{i_T \in \{0,1\}^M} (i_T)_k \mathrm{Tr}\left[\rho_{A_{i_T}}\right]. \tag{3.17}$$

Asking for all qubits to be the same is equivalent to equating to zero the expression

$$\langle 1|(\rho'_\alpha - \rho'_\gamma)|1\rangle = \sum_{i_T \in \{0,1\}^M} ((i_T)_\alpha - (i_T)_\gamma) \mathrm{Tr}\left[\rho_{A_{i_T}}\right]. \tag{3.18}$$

Since for $(i_T)_\alpha = (i_T)_\gamma = 0, 1$ everything vanishes, and by requiring $\langle 1|(\rho'_\alpha - \rho'_\gamma)|1\rangle = 0$, one obtains:

$$\sum_{\substack{i_T \in \{0,1\}^M \\ ((i_T)_\alpha, (i_T)_\gamma) = (1,0)}} \mathrm{Tr}\left[\rho_{A_{i_T}}\right] = \sum_{\substack{i_T \in \{0,1\}^M \\ ((i_T)_\alpha, (i_T)_\gamma) = (0,1)}} \mathrm{Tr}\left[\rho_{A_{i_T}}\right]. \tag{3.19}$$

This generalizes the condition found for $M = 2$ to an arbitrary M, and it generates a set of $M(M-1)$ conditions on 2^M unknown variables $\mathrm{Tr}\left[\rho_{A_{i_T}}\right]$, for $i_T \in \{0,1\}^M$.
Since the sum spans over all possible values of $i_T \in \{0,1\}^M$ with fixed values on the α and γ digits, and since these two digits are constrained to have Hamming weight equal to 1, a solution is given by equating each term of the sum with the correspondent on the other side of the equation, leading to the criteria: two blocks that have the same Hamming weight should have the same trace. Mathematically, it reads

$$\mathrm{Tr}\left[\rho_{A_i}\right] = \mathrm{Tr}\left[\rho_{A_j}\right] \qquad \forall\ i, j \text{ such that } w(i) = w(j) \tag{3.20}$$

where $w(i)$ gives the Hamming weight of the string of M digits "i".
From a physical perspective, this is equivalent for the degenerate states of the M target qubits to have equal probability, since they are identical. Moreover, this means that it is necessary for the final configuration to maintain a binomial symmetry: the eigenstates of the final density matrix of the target system will have degeneracy $\binom{M}{i}$, where i is the number of excited target qubits. A graphical representation of this condition is shown in Figures 3.2 and 3.3, in which we can explicitly see the symmetric nature of the problem, which becomes for all means a partitioning problem, as we will discuss in Section 3.2.

3.2 On the unique temperature condition

To ensure that all M target qubits reach an identical final state (and thus a common effective temperature), the reduced density matrix of the target system, $\rho'_T = \mathrm{Tr}_A[\rho']$, must exhibit a specific symmetry. As derived in Equation 3.19, this requirement is satisfied if the traces of the ancillary blocks $\rho_{A_{i_T}}$ depend solely on the Hamming weight $w(i_T)$ of the target configuration $i_T \in \{0,1\}^M$.

Mathematically, this implies that for any two target configurations i, j with $w(i) = w(j)$, we must have:

$$\mathrm{Tr}[\rho_{A_i}] = \mathrm{Tr}[\rho_{A_j}]. \tag{3.21}$$

Under the action of an energy-minimizing unitary operator, which populates the states of the global system in increasing order of energy (from the ground state $i = 0$ to N), this condition translates into a non-trivial multiset partition problem.

In this section, we begin with the search for solutions of such a problem by studying in detail the mathematical setting behind the unique temperature requirement. Then, we consider the case in which the spectral structure of the initial state does not allow to fulfill the unique temperature requirement, and we show that, by applying an additional unitary operation, we can recover a configuration that allows the existence of a unique local temperature.

3.2.1 Solutions for the Partition Problem

The initial system consists of 2^N eigenstates, where the i-th energy level has a degeneracy given by the binomial coefficient $\binom{N}{i}$. To achieve the desired

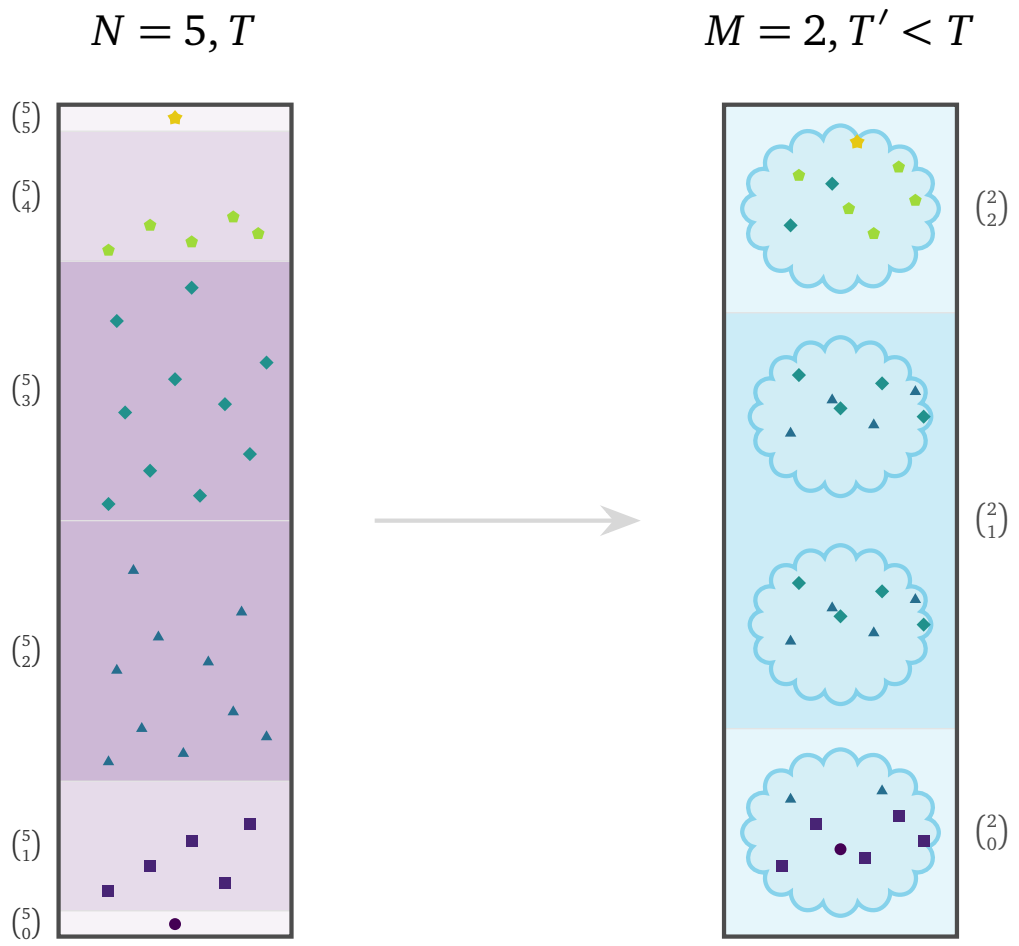

Figure 3.2: Here we show a graphic interpretation of the condition 3.19 in the specific case with $N = 5$ intial qubits and $M = 2$ target. In the left side we can see the spectral structure of the initial thermal state ρ, while in the right side the final spectra of the target qubits state ρ'_T. Let us focus on the initial state: the density matrix eigenvalues of a 5 identical qubits system have binomial degeneracy. The eigenvalues are represented as geometrical object - circles, squares, triangles,..- such that elements with the same shape represent eigenvalues that have the same value. For clarity, for $i = 0$ the circle represents the unique eigenvalue P_0^5, for $i = 1$ the squares represent the 5-degenerate eigenvalues $P_0^4 P_1$, and so on. In the right side clouds represent eigenvalues of the final density matrix ρ'_T: the cloud in the bottom represents eigenvalue refered to eigenstate $|00\rangle$, and it given by the sum of the element inside the cloud. The same holds with the other clouds, for states $|01\rangle$, $|10\rangle$ and $|11\rangle$. With some fantasy, we can think of the clouds as a Trace operators that act on the diagonal matrix build with eigenvalues contained inside the cloud (this is exactly what they are doing on the matrix of the ancillary system via Equation 3.16). As we can see, here states $|01\rangle$ and $|10\rangle$ have same probability: $N = 5$ and $M = 2$ guarantee a unique final temperature.

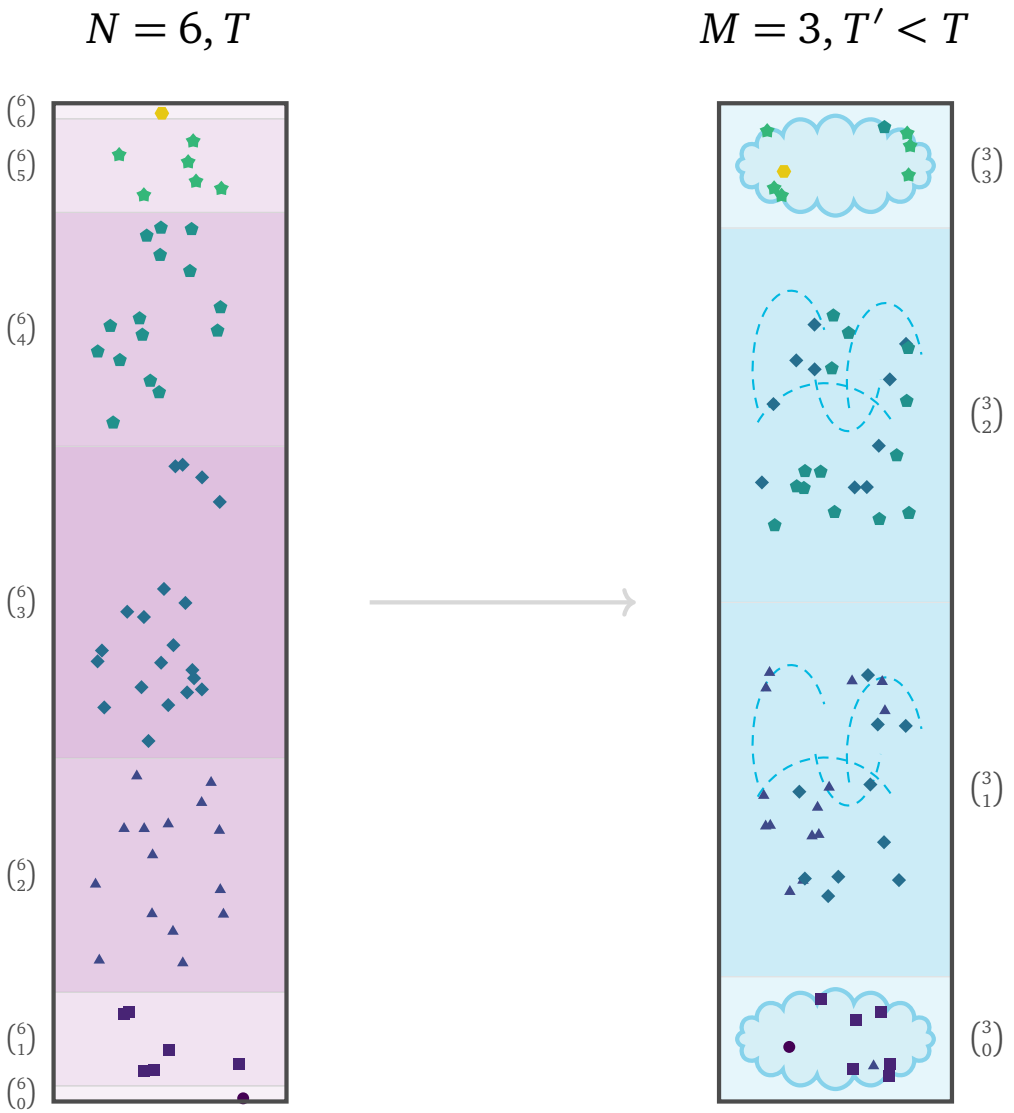

Figure 3.3: Here we follow the line of Figure 3.2, but with $N = 6$ and $M = 3$. In this particular case, a perfect matching of eigenvalues is not possible: we cannot reach a unique temperature final configuration. Indeed, in the ground state block of the target $\binom{3}{0}$ are contained 1 eigenvalue from the first block in the left $\binom{6}{0}$, all 6 eigenvalues of the initial second degenerate block $\binom{6}{1}$, and 1 of the third block $\binom{6}{2}$. Thus, for the second 3-denerate block $\binom{3}{1}$, we have to share $15-1=14$ eigenvalues of the second block $\binom{6}{2}$ and half of the central block $\binom{6}{3}$ - wiche are $20/2=10$. Clearly, both this values are not divisible by 3, hence they cannot be shared within the three blocks.

symmetry, these 2^N eigenvalues must be distributed among 2^M blocks, each of dimension 2^{N-M}. These blocks are grouped into $M+1$ equivalence classes based on their Hamming weight $w \in \{0,\dots,M\}$, where each class contains $\binom{M}{w}$ blocks

A rearrangement is deemed physically feasible if and only if each block within the same Hammingclass w can be assigned an identical spectrum of eigenvalues. Since eigenvalues belonging to the same degenerate subspace $\binom{N}{i}$ are indistinguishable, the problem reduces to verifying the divisibility of the available multiplicities.

Algorithmic Formulation of the Problem

In order to understand the occurrence of solutions to this partition problem, we show how to implement an algorithm which, given as input the binary couple (N,M), gives as an outcome a yes/no statement based on whether the partition is possible or not.

The logical flow can be decomposed into the following conceptual steps:

1. **Initial Configuration**: The initial state is characterized by a set of energy levels $i \in [0,N]$, each associated with a degeneracy $m_i = \binom{N}{i}$. In our algorithmic framework, these multiplicities represent a set of identical eigenvalues that must be distributed. Simultaneously, the target system's blocks have size $L = 2^{N-M}$, which dictates the total capacity of each ancillary block $\rho_{A_{i_T}}$.

2. **Grouping by Symmetry Classes**: The algorithm does not treat each of the 2^M blocks individually. Instead, it groups them into $M+1$ equivalence classes based on their Hamming weight w. This reflects the physical requirement that configurations with the same weight must be locally indistinguishable. For a given class w, the total number of blocks to be filled simultaneously is $K_w = \binom{M}{w}$, and the total capacity required for the class is $C_w = K_w \times L$.

3. **Energy-Ordered Allocation**: To minimize the final energy of the target qubits, the algorithm follows a greedy filling strategy. It populates the Hammingclasses in increasing order (from $w = 0$ to $w = M$) and draws eigenvalues from the reservoir starting from the lowest energy index ($i = 0$ to N). This ensures that the highest eigenvalues (lowest i) are assigned to the target states with the lowest Hamming weight.

4. **Symmetry Consistency Check**: As the algorithm draws a quantity n_{take} of eigenvalues of type i to fill a class w, it encounters the fundamental

constraint of the problem. For the K_w blocks in the class to be identical, every eigenvalue of type i must be distributed equally among them. This leads to the Condition:

$$n_{take} \pmod{K_w} \equiv 0 \tag{3.22}$$

This step represents the mathematical core of the feasibility check. If n_{take} is not a multiple of K_w, it implies that a perfectly symmetric distribution of the discrete spectrum is impossible, leading to a failure of the unique temperature condition for that specific (N, M) configuration.

5. **Iteration**: Upon a successful check, the reservoir is updated ($m_i = m_i - n_{take}$) and the class requirement is reduced. The process repeats until all Hammingclasses are fully populated. If the algorithm reaches the final class $w = M$ without violating Condition 3.22, the rearrangement is declared feasible.

By framing the algorithm in this manner, we realize that the impossibility of a unique temperature is not due to a lack of states, but rather to a "broken symmetry" that arises when the discrete degeneracies of the initial system cannot be partitioned into the fixed-size blocks required by the target system's geometry.

Despite the highly constrained structure of the partition problem, it is remarkable to observe that there is a counterintuitive richness of the couples (N, M) that permit an effective partition. This is what is shown in Table 3.1, where for each number of target qubits $M \in [2, 10]$ are shown the possible values of N that guarantee the feasibility of the partition.

From the table we notice, for small values of M, that various "island of feasibility" exist, with dimensions that decrease with increasing M. While the existence of feasible numbers N for $M = 2$ was somehow expected, it is remarkable to see that also $M = 3$, $M = 4$, and $M = 5$ present a quite abundant occurrence of combinations (N, M) that fulfill the partition.
The number $M = 6$ acts here as a threshold value: the binomial structure imposes now constraints that are too strong to be overcome. This remains valid for higher values of M, even if it is curious to notice the presence of some outliers for $M = 7, 8$, represented respectively by the numbers $N = 55, 67$: the number theoretic nature of this partitioning problem makes it impossible to predict precisely the behavior for asymptotic regimes.

3.2.2 Off diagonal terms restore unique temperature

Even if the unique temperature requirement cannot be fulfilled, all is not lost.

Target M	Feasible System Sizes (N)
$M = 2$	5–7, 9–14, 17–29, 33–59, 65–121
$M = 3$	9–14, 27–47, 63, 81–128
$M = 4$	10, 34, 35, 49–51, 66–68, 81–83, 97–112
$M = 5$	25–28, 33–39, 75–83
$M = 6$	
$M = 7$	55
$M = 8$	67
$M = 9$	
$M = 10$	

Table 3.1: Global mapping of unique temperature cooling feasibility. The values of $N \in [M+2, 128]$ represent the total system sizes for which a symmetric rearrangement of the spectrum is possible. Here we do not consider the case $M = N - 1$, as it always fullfill the condition but does not lead to cooling (see Section 3.3). Note the isolation of feasible N values for $M \geq 6$, where symmetry constraints become dominant.

Indeed, here we consider the specific case with $N = 4$ and $M = 2$ and show that we can recover locally identical states, at the cost of introducing off diagonal terms.

Example for $N = 4$, $M = 2$

Consider the final state density matrix (written with basis vectors ordered with K_2 - the Hamiltonian of target qubits) that one obtains by only requiring minimal energy for the $M = 2$ qubits, call it ρ_{U_0}:

$$\rho_{U_0} = \left[\begin{array}{cccc|cccc|cccc|cccc} P_0^4 & 0 & 0 & 0 & & & & & & & & & & & & \\ 0 & P_0^3P_1 & 0 & 0 & & & & & & & & & & & & \\ 0 & 0 & P_0^3P_1 & 0 & & & & & & & & & & & & \\ 0 & 0 & 0 & P_0^3P_1 & & & & & & & & & & & & \\ \hline & & & & P_0^3P_1 & 0 & 0 & 0 & & & & & & & & \\ & & & & 0 & P_0^2P_1^2 & 0 & 0 & & & & & & & & \\ & & & & 0 & 0 & P_0^2P_1^2 & 0 & & & & & & & & \\ & & & & 0 & 0 & 0 & P_0^2P_1^2 & & & & & & & & \\ \hline & & & & & & & & P_0^2P_1^2 & 0 & 0 & 0 & & & & \\ & & & & & & & & 0 & P_0^2P_1^2 & 0 & 0 & & & & \\ & & & & & & & & 0 & 0 & P_0^2P_1^2 & 0 & & & & \\ & & & & & & & & 0 & 0 & 0 & P_0P_1^3 & & & & \\ \hline & & & & & & & & & & & & P_0P_1^3 & 0 & 0 & 0 \\ & & & & & & & & & & & & 0 & P_0P_1^3 & 0 & 0 \\ & & & & & & & & & & & & 0 & 0 & P_0P_1^3 & 0 \\ & & & & & & & & & & & & 0 & 0 & 0 & P_1^4 \end{array}\right] \tag{3.23}$$

Here, we cannot build, even in principle, a final thermal state for the M qubits: in the central blocks there are two eigenvalues, $P_0^3P_1$ and $P_0P_1^3$, which appear only once. Thus, it is impossible to distribute them over the two blocks and we are left with no possibility of building a final state with same temperature. But what if there exists some transformation that gives us the state:

$$\rho_{U_0'} = \left[\begin{array}{cccc|cccc|cccc|cccc} P_0^4 & 0 & 0 & 0 & & & & & & & & & & & & \\ 0 & P_0^3P_1 & 0 & 0 & & & & & & & & & & & & \\ 0 & 0 & P_0^3P_1 & 0 & & & & & & & & & & & & \\ 0 & 0 & 0 & P_0^3P_1 & & & & & & & & & & & & \\ \hline & & & & a & b & 0 & 0 & & & & & & & & \\ & & & & b^* & a & 0 & 0 & & & & & & & & \\ & & & & 0 & 0 & P_0^2P_1^2 & 0 & & & & & & & & \\ & & & & 0 & 0 & 0 & P_0^2P_1^2 & & & & & & & & \\ \hline & & & & & & & & P_0^2P_1^2 & 0 & 0 & 0 & & & & \\ & & & & & & & & 0 & P_0^2P_1^2 & 0 & 0 & & & & \\ & & & & & & & & 0 & 0 & c & d & & & & \\ & & & & & & & & 0 & 0 & d^* & c & & & & \\ \hline & & & & & & & & & & & & P_0P_1^3 & 0 & 0 & 0 \\ & & & & & & & & & & & & 0 & P_0P_1^3 & 0 & 0 \\ & & & & & & & & & & & & 0 & 0 & P_0P_1^3 & 0 \\ & & & & & & & & & & & & 0 & 0 & 0 & P_1^4 \end{array}\right]. \tag{3.24}$$

For such a state, it would be possible to reorder the eigenvalues of the central blocks to have equal partial trace! Indeed, that state would be:

$$\rho' = \left[\begin{array}{cccc|cc|cc|cc|cccc} P_0^4 & 0 & 0 & 0 & & & & & & & & & & \\ 0 & P_0^3P_1 & 0 & 0 & & & & & & & & & & \\ 0 & 0 & P_0^3P_1 & 0 & & & & & & & & & & \\ 0 & 0 & 0 & P_0^3P_1 & & & & & & & & & & \\ \hline & & & & a & & & & & & & & & \\ & & & & & d & & & & & & & & \\ & & & & & & P_0^2P_1^2 & & & & & & & \\ & & & & & & & P_0^2P_1^2 & & & & & & \\ \hline & & & & & & & & P_0^2P_1^2 & & & & & \\ & & & & & & & & & P_0^2P_1^2 & & & & \\ & & & & & & & & & & a & & & \\ & & & & & & & & & & & d & & \\ \hline & & & & & & & & & & & & P_0P_1^3 & 0 & 0 & 0 \\ & & & & & & & & & & & & 0 & P_0P_1^3 & 0 & 0 \\ & & & & & & & & & & & & 0 & 0 & P_0P_1^3 & 0 \\ & & & & & & & & & & & & 0 & 0 & 0 & P_1^4 \end{array}\right], \quad (3.25)$$

where, in general, the permutation of central blocks eigenvalues can move the off diagonal terms in the central blocks (for this reason, we left it blanck - they are not all equal to zero). In this particular case, the operation can be done via a Hadamard gate on a particular subspace.

Indeed, consider the subspace generated by the state vectors $|0100\rangle$ and $|1000\rangle$. Applying a transformation that is isomorphic to a Hadamard gate on this subspace while acting as the identity on the other state vectors, we get:

$$\begin{aligned} |0100\rangle &\to \frac{1}{\sqrt{2}}(|0100\rangle + |1000\rangle), \\ |1000\rangle &\to \frac{1}{\sqrt{2}}(|0100\rangle - |1000\rangle). \end{aligned} \quad (3.26)$$

The correspondent block of the density matrix becomes:

$$\begin{pmatrix} P_0^3P_1 & 0 \\ 0 & P_0^2P_1^2 \end{pmatrix} \to \frac{1}{2}\begin{pmatrix} (P_0^3P_1 + P_0^2P_1^2) & (P_0^3P_1 - P_0^2P_1^2) \\ (P_0^3P_1 - P_0^2P_1^2) & (P_0^3P_1 + P_0^2P_1^2) \end{pmatrix}. \quad (3.27)$$

The same can be proven for the subspace generated by state vectors $|0111\rangle$ and $|1011\rangle$. We thus recover a final state that exhibits unique temperature, at the cost of introducting off diagonal terms. Moreover, the final excited state population will be the average of the final excited state populations of single target qubits without the mixing procedure. Indeed, if we compute the final excited state population without this procedure, we have (see Equation 3.13 applied to the density matrix ρ_{U_0}):

$$\begin{aligned} \langle 1|\rho_1'|1\rangle &= 3P_0^2P_1^2 + 4P_0P_1^3 + P_1^4 \\ \langle 1|\rho_2'|1\rangle &= P_0^3P_1 + 3P_0^2P_1^2 + 3P_0P_1^3 + P_1^4. \end{aligned} \quad (3.28)$$

Meanwhile, by adding the Hadamard gates we obtain:

$$\langle 1|\rho_1'|1\rangle = \langle 1|\rho_2'|1\rangle = \frac{(P_0^3P_1 + P_0P_1^3)}{2} + 3P_0^2P_1^2 + 3P_0P_1^3 + P_1^4 \tag{3.29}$$

Thus, the Hadamard gates operate as a symmetrization of the degenerate blocks.

Here, we considered an example for $N = 4$ and $M = 2$, but is this a general procedure?

General Case: QFT in action

In the general case, the Quantum Fourier Transform enters the game. In Section 2.1 we have shown that the action of a QFT on a diagonal state yields a final state whose diagonal is made of degenerate elements that amount to the mean of the eigenvalues. This is exactly what we need.

Consider, as an example, the state obtained for dynamic cooling of $M = 3$ qubits:

$$\rho' = \begin{bmatrix} \rho_{A_{000}} & & & & & & & \\ & \rho_{A_{001}} & & & & & & \\ & & \rho_{A_{010}} & & & & & \\ & & & \rho_{A_{100}} & & & & \\ & & & & \rho_{A_{011}} & & & \\ & & & & & \rho_{A_{101}} & & \\ & & & & & & \rho_{A_{110}} & \\ & & & & & & & \rho_{A_{111}} \end{bmatrix}, \tag{3.30}$$

where, in addition to the blocks of ancillary systems, we inserted the blocks of equal Hamming weight subspaces. We denote these blocks by ρ_{w_k}, with "w_k"

referring to the degenerate subspace of states with Hamming weight $w = k$. The formal definition for these is:

$$\rho_{w_k} := \bigoplus_{i=1}^{\binom{M}{k}} \rho_{A_i}, \tag{3.31}$$

where $i \in \{0,1\}^M$ are the strings with Hamming weight $w = k$, and $\bigoplus$ denotes the direct sum. Let N be the initial number of qubits, such that the unique temperature condition cannot be fulfilled: then there does not exist a unitary operation such that $\mathrm{Tr}\left[\rho_{A_i}\right] = \mathrm{Tr}\left[\rho_{A_j}\right]$ for $w(i) = w(j)$.

This situation can be recovered quite easily by applying a QFT on the degenerate K_M subspaces: considering the density matrix above, ρ', a QFT must be applied on the two blocks ρ_{w_1}, ρ_{w_2}. Indeed, the final symmetrized state will be

$$\rho'_{sym} = \left[\begin{array}{c|c|c|c} \rho_{A_{000}} & & & \\ \hline & \mathscr{F}\rho_{w_1}\mathscr{F}^\dagger & & \\ \hline & & \mathscr{F}\rho_{w_2}\mathscr{F}^\dagger & \\ \hline & & & \rho_{A_{111}} \end{array}\right]. \tag{3.32}$$

For the property of QFT introduced in Section 2.1, the two blocks will now have degenerate diagonal elements that coincide with the mean of the eigenvalues of the respective matrices ρ_{w_1} and ρ_{w_2}.

The new density matrix ρ'_{sym} ensures a unique temperature for the target qubits.

Indeed, consider the factorized form of the state:

$$\rho'_{sym} = \sum_{i,j\in\{0,1\}^M} |i\rangle\langle j| \otimes \rho_{A_{|i\rangle\langle j|}}, \tag{3.33}$$

where the density matrix allows the presence of off diagonal terms, represented by the matrices $\rho_{A_{|i\rangle\langle j|}}$ in the state space of the ancillary system. In particular, since the QFT acts only on the degenerate subspaces, $\rho_{A_{|i\rangle\langle j|}} \neq 0$ if and only if $w(i) = w(j)$. For clarity, we show the representation of the matrix ρ'_{sym} for $M = 3$:

$$\rho'_{sym} = \left[\begin{array}{c|ccc|ccc|c} \rho_{A_{000}} & & & & & & & \\ \hline & \rho_{A_{001}} & \rho_{A_{|001\rangle\langle 010|}} & \rho_{A_{|001\rangle\langle 100|}} & & & & \\ & \rho_{A_{|010\rangle\langle 001|}} & \rho_{A_{010}} & \rho_{A_{|010\rangle\langle 100|}} & & & & \\ & \rho_{A_{|100\rangle\langle 001|}} & \rho_{A_{|100\rangle\langle 010|}} & \rho_{A_{100}} & & & & \\ \hline & & & & \rho_{A_{011}} & \rho_{A_{|011\rangle\langle 101|}} & \rho_{A_{|011\rangle\langle 110|}} & \\ & & & & \rho_{A_{|101\rangle\langle 011|}} & \rho_{A_{101}} & \rho_{A_{|101\rangle\langle 110|}} & \\ & & & & \rho_{A_{|110\rangle\langle 011|}} & \rho_{A_{|110\rangle\langle 101|}} & \rho_{A_{110}} & \\ \hline & & & & & & & \rho_{A_{111}} \end{array}\right], \tag{3.34}$$

where, for coherence of notation, we define $\rho_{A_{|i\rangle\langle i|}} := \rho_{A_i}$. The target system final state follows from the partial trace over the ancillary system:

$$(\rho'_{sym})_T = \sum_{i,j\in\{0,1\}^M} \mathrm{Tr}\left[\rho_{A_{|i\rangle\langle j|}}\right] |i\rangle\langle j| . \tag{3.35}$$

Then, the state of the k-th target qubit is given by partial tracing all the target qubits apart from the k-th:

$$(\rho'_{sym})_k = \sum_{l\in\{0,1\}^{M\setminus\{k\}}} \langle l| (\rho'_{sym})_T |l\rangle . \tag{3.36}$$

Explicitly, we have:

$$
\begin{aligned}
(\rho'_{sym})_k &= \sum_{l\in\{0,1\}^{M\setminus\{k\}}} \langle l| \left[\sum_{i,j\in\{0,1\}^M} \mathrm{Tr}\left[\rho_{A_{|i\rangle\langle j|}}\right] |i\rangle\langle j| \right] |l\rangle = \\
&= \sum_{l\in\{0,1\}^{M\setminus\{k\}}} \sum_{i,j\in\{0,1\}^M} \mathrm{Tr}\left[\rho_{A_{|i\rangle\langle j|}}\right] \langle l|i\rangle\langle j|l\rangle = \\
&= \sum_{i_k,j_k\in\{0,1\}} |i_k\rangle\langle j_k| \sum_{l\in\{0,1\}^{M\setminus\{k\}}} \mathrm{Tr}\left[\rho_{A_{|l\cup i_k\rangle\langle l\cup j_k|}}\right].
\end{aligned} \tag{3.37}
$$

But, as previously claimed, $\rho_{A_{|i\rangle\langle j|}} \neq 0$ if and only if $w(i) = w(j)$: here, the elements $\rho_{A_{|l\cup i_k\rangle\langle l\cup j_k|}}$ are different from zero if and only if $i_k = j_k$, which means that they are both either "0" or "1". The final state of the k-th target becomes:

$$
\begin{aligned}
(\rho'_{sym})_k &= \sum_{i_k\in\{0,1\}} |i_k\rangle\langle i_k| \sum_{l\in\{0,1\}^{M\setminus\{k\}}} \mathrm{Tr}\left[\rho_{A_{|l\cup i_k\rangle\langle l\cup i_k|}}\right] = \\
&= \sum_{\substack{l\in\{0,1\}^M \\ l_k=0}} \mathrm{Tr}\left[\rho_{A_{|l\rangle\langle l|}}\right] |0\rangle\langle 0| + \sum_{\substack{l\in\{0,1\}^M \\ l_k=1}} \mathrm{Tr}\left[\rho_{A_{|l\rangle\langle l|}}\right] |1\rangle\langle 1|.
\end{aligned} \tag{3.38}
$$

Isolating the excited state population:

$$
\langle 1|(\rho'_{sym})_k|1\rangle = \sum_{\substack{l\in\{0,1\}^M \\ l_k=1}} \mathrm{Tr}\left[\rho_{A_{|l\rangle\langle l|}}\right] = \sum_{l\in\{0,1\}^M} (l_k)\mathrm{Tr}\left[\rho_{A_l}\right], \tag{3.39}
$$

where we used the notation introduced before $\rho_{A_{|j\rangle\langle j|}} := \rho_{A_j}$.
This is completely identical to Equation 3.17, yielding a unique temperature condition that is exactly the same as that given by Equation 3.19. By taking again the solution

$$
\mathrm{Tr}\left[\rho_{A_i}\right] = \mathrm{Tr}\left[\rho_{A_j}\right] \qquad \forall\ i,j \text{ such that } w(i) = w(j), \tag{3.40}
$$

we have that the unique temperature is always guaranteed by construction, since now, thanks to the QFTs, we have diagonal blocks with diagonal elements averaged with eigenvalues of the initial blocks with same Hamming weight.

Note, while the graphical representation shows the case $M = 3$, that the calculations are general and provide a proof for the case with arbitrary M.

Additionally, we observe that this procedure, despite being the most general, is not optimal in terms of resources. Indeed, as seen in the example with $N = 4$ and $M = 2$ it is not necessary, in general, to symmetrize all subspaces with degenerate Hamming weight, it would be enough to symmetrize subspaces that contain eigenvalues that are not divisible by the number of degenerate blocks. This could be done specifically once all parameters N and M have been specified, making a general procedure with minimal resources impossible to formalize.

3.3 Cooling Temperature

Suppose that we are dealing with a system with N, M such that it is possible to fulfill condition 3.19, what final temperature are we able to reach? Under this assumption the M target qubits have locally the same temperature, thus it is sufficient to compute the temperature of one of them to know the temperature of each one. Moreover, the temperature of one qubit is given by the relation with the excited state occupation probability $P_1 = 1/(1 + e^{\beta\hbar\omega})$.

3.3.1 Two target qubits

For two target qubits, i.e. $M = 2$, the reduced states are given by Equation 3.13. Since we are considering the case in which the condition of unique temperature is fulfilled, we can write

$$\mathrm{Tr}\left[\rho_{A_{01}}\right] = \mathrm{Tr}\left[\rho_{A_{10}}\right] = \frac{1}{2}\left\{\mathrm{Tr}\left[\rho_{A_{01}}\right] + \mathrm{Tr}\left[\rho_{A_{10}}\right]\right\}. \tag{3.41}$$

Using this equation, the excited state population becomes:

$$P_1' = \frac{1}{2}\left\{\mathrm{Tr}\left[\rho_{A_{01}}\right] + \mathrm{Tr}\left[\rho_{A_{10}}\right]\right\} + \mathrm{Tr}\left[\rho_{A_{11}}\right], \tag{3.42}$$

with

$$\begin{aligned}
\mathrm{Tr}\left[\rho_{A_{11}}\right] &= \sum_{k=N-\xi_2^\star+1}^{N} \binom{N}{k} P_1^k (1-P_1)^{N-k} + \alpha_{A_{11}} P_1^{N-\xi_2^\star} (1-P_1)^{\xi_2^\star}, \\
\mathrm{Tr}\left[\rho_{A_{01}}\right] + \mathrm{Tr}\left[\rho_{A_{10}}\right] + \mathrm{Tr}\left[\rho_{A_{11}}\right] &= \sum_{k=\xi_2^\star+1}^{N} \binom{N}{k} P_1^k (1-P_1)^{N-k} + \\
&\quad + \left\{\binom{N}{\xi_2^\star} - \alpha_{A_{00}}\right\} P_1^{\xi_2^\star} (1-P_1)^{N-\xi_2^\star},
\end{aligned} \tag{3.43}$$

where we defined

$$\xi_2^\star := \text{argmax}_\xi \left\{ \sum_{k=0}^{\xi-1} \binom{N}{k} \leq 2^{N-2} \right\}, \tag{3.44}$$

$$\alpha_{A_{11}} := \left\{ 2^{N-2} - \sum_{k=N-\xi_2^\star+1}^{N} \binom{N}{k} \right\}, \tag{3.45}$$

$$\alpha_{A_{00}} := \left\{ 2^{N-2} - \sum_{k=0}^{\xi_2^\star-1} \binom{N}{k} \right\}. \tag{3.46}$$

These have been computed according to the action of the unitary $\mathscr{U}$: for $\text{Tr}\left[\rho_{A_{11}}\right]$ we counted the 2^{N-2} smallest probabilities and, vice versa, the highest probabilities for $\text{Tr}\left[\rho_{A_{00}}\right]$. The coefficients α_{A_i} are needed to count the states in excess.
In Figure 3.4, we plot the function given by Equation 3.42 for different values of N such that the unique temperature condition is fulfilled. We compare it with the parallel action of two single qubit cooling algorithms. In particular, we consider a number N of available qubits at the same temperature T as resources, and we compare how much we can cool two target qubits at the same temperature in the two different ways. As we can see in Figure 3.4, single shot cooling of two qubits is almost always convenient. This is so for the following reasons:

- while for our algorithm all qubits will be used, for the parallel action of single qubit cooling only the integer part of $N/2$ will be used (we need equal parameters to have same final temperature): when N is odd we lose a qubit as soon as we start.
- single qubit cooling algorithms fulfill property 2.35: if we want to use all qubits, we need to start from an even number N such that $N/2$ is odd. For N that do not fulfill this condition, we lose resources.

Low Temperature regime

Moreover, from Equation 3.42, we can extract a low temperature estimate. Low temperature translates into low P_1: we take the Taylor expansion around the value $P_1 = 0$:

$$P_1'(P_1,N) = \sum_{k=0}^{\infty} \frac{1}{k!} \frac{\partial^k P_1'(P_1,N)}{\partial P_1^k}\bigg|_{P_1=0} P_1^k. \tag{3.47}$$

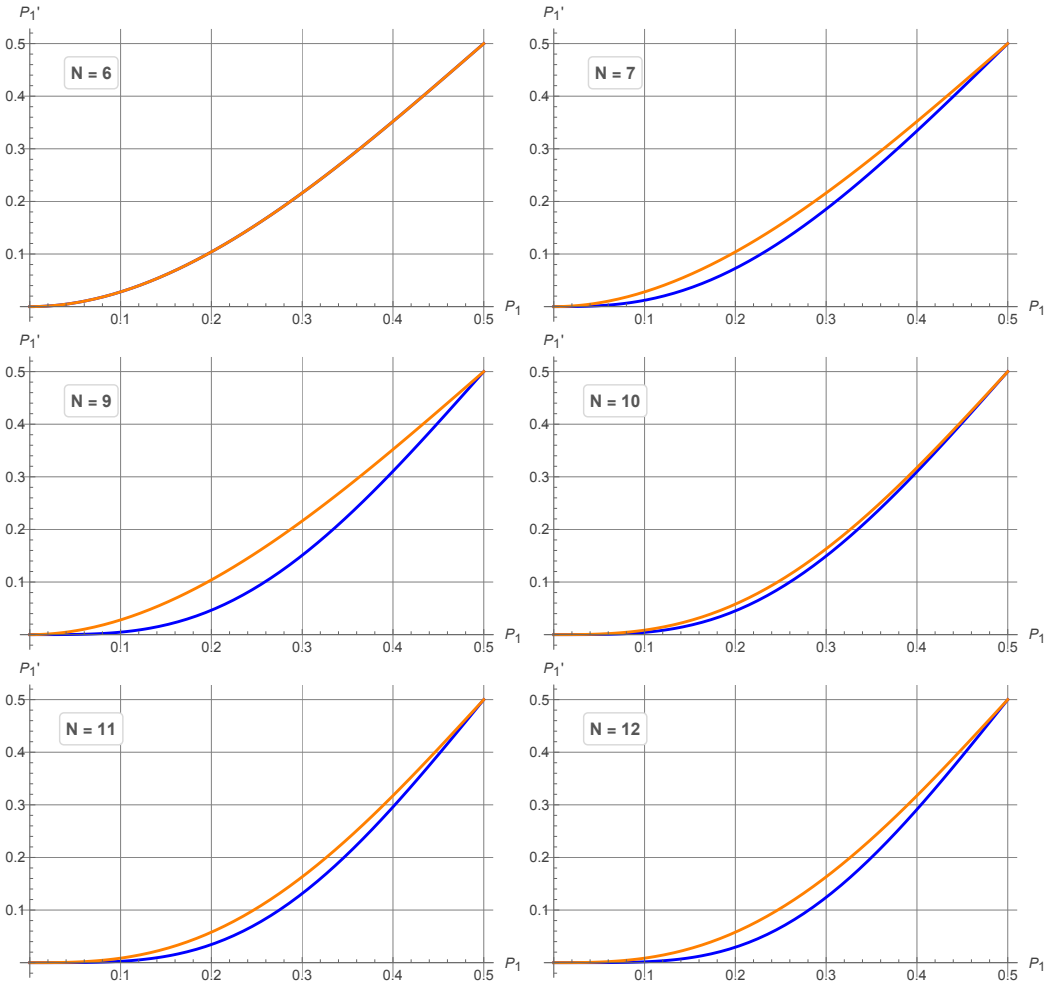

Figure 3.4: Plots of the function $P_1'(N, P_1)$ given in Equation 3.42, in blue, compared with Equation 2.32 for $N = N/2$, in orange. In the top are represented the cases with $N = 6$ (left) and $N = 7$ (right): for $N = 6$ the temperature reached is the same for both algorithms. This is connected to the fact that in the parallel of single qubit cooling we use $N/2 = 3$ qubits: we do not lose qubit at the start because N is even and we do not later beacuse $N/2$ is odd. For the same reason is easy to accept the fact that for $N = 7$ the single shot cooling of two qubits win. Also for $N = 9$ (center-left) single shot cooling wins: 1 qubit is lost since N is odd, and two additional qubits are lost since $N/2$ is even. Note that we did not report $N = 8$ since in that case is it is not possible to build a unitary that gives unique temperature. It is curious to see that, for $N = 10$ (center-right), we still have a better performance from the single shot algorithm. In the bottom we report the case $N = 11$ (left) and $N = 12$ (right), in both case single shot algorithm has a better performance: in this case we can explain that with the loss of qubits, since $N = 11$ is odd and $N = 12$ is such that $N/2 = 6$ is even.

The explicit formula for $P_1'(P_1,N)$ is

$$P_1'(P_1,N)=\frac{1}{2}\left\{\sum_{k=\xi_2^\star+1}^{N}\binom{N}{k}P_1^k(1-P_1)^{N-k}+\left\{\binom{N}{\xi_2^\star}-\alpha_{A_{00}}\right\}P_1^{\xi_2^\star}(1-P_1)^{N-\xi_2^\star}\right\}+$$
$$+\frac{1}{2}\left\{\sum_{k=N-\xi_2^\star+1}^{N}\binom{N}{k}P_1^k(1-P_1)^{N-k}+\alpha_{A_{11}}P_1^{N-\xi_2^\star}(1-P_1)^{\xi_2^\star}\right\}, \tag{3.48}$$

which, at lowest order, becomes

$$P_1'(P_1,N)=\frac{1}{2}\left\{\binom{N}{\xi_2^\star+1}P_1^{\xi_2^\star+1}+\left\{\binom{N}{\xi_2^\star}-\alpha_{A_{00}}\right\}P_1^{\xi_2^\star}\right\}+O(P_1^{\xi_2^\star+2}). \tag{3.49}$$

We are now able to find an estimate of the cooling temperature in the low T regime: consider the low temperature approximation $P_1\approx e^{-\beta\hbar\omega}$, $P_1'\approx e^{-\beta'\hbar\omega}$. Under this approximation, for all $C,l<\infty$ such that $P_1'=CP_1^l$, we have $\beta\hbar\omega=-\log(C)+l\beta'\hbar\omega$ and, since $\beta,\beta'\to\infty$ and C is finite, we get $\beta'\simeq l\beta$ which translates into

$$T'\simeq\frac{T}{l}. \tag{3.50}$$

In Equation 3.49, the degree is either $\xi_2^\star$ or $\xi_2^\star+1$:

$$T'\simeq\begin{cases}\dfrac{T}{\xi_2^\star} & \text{if } \binom{N}{\xi_2^\star}\neq\alpha_{A_{00}},\\[2ex] \dfrac{T}{\xi_2^\star+1} & \text{otherwise.}\end{cases} \tag{3.51}$$

In the following paragraph, we will derive a similar result for generic M, and we will give a more explicit bound based on the definition of $\xi_2^\star$.

3.3.2 M target qubits

Now, we generalize to arbitrary number of target qubits M. We keep the assumption for which it is possible, in principle, to have a unique final temperature and we search for the minimal temperature reachable. The excited state

population of the k-th target qubit is given by Equation 3.17:

$$\langle 1|\rho'_k|1\rangle = P'_1 = \sum_{\substack{i_T\in\{0,1\}^M \\ (i_T)_k=1}} \mathrm{Tr}\Big[\rho_{A_{i_T}}\Big]. \tag{3.52}$$

We can insert the unique temperature condition 3.19 in the following way: given a string j with Hamming weight $w = w(j)$, then one has

$$\mathrm{Tr}\Big[\rho_{A_j}\Big] = \frac{1}{\binom{M}{w}} \sum_{\substack{\beta\in\{0,1\}^M \\ w(\beta)=w}} \mathrm{Tr}\Big[\rho_{A_\beta}\Big]. \tag{3.53}$$

Indeed, since the condition tells us that states with same Hamming weight have equal probability, this means that the probability of one of them is the mean of all the probabilities (after all, they all amount the same!).
To sum only the terms with "1" as first digit, one needs to consider exactly $\binom{M-1}{w-1}$ traces, since we are considering all possible strings of M qubits with weight w constrained to have first digit equal to 1, hence $M-1$ digits with weight $w-1$. The sum must span over all weights from $w-1=0$ to $w-1=M-1$. Hence, we obtain:

$$P'_1 = \sum_{i=1}^{M} \frac{\binom{M-1}{i-1}}{\binom{M}{i}} \sum_{\substack{j\in\{0,1\}^M \\ w(j)=i}} \mathrm{Tr}\Big[\rho_{A_j}\Big] = \sum_{i=1}^{M} \frac{i}{M} \sum_{\substack{j\in\{0,1\}^M \\ w(j)=i}} \mathrm{Tr}\Big[\rho_{A_j}\Big]. \tag{3.54}$$

Low Temperature regime

Although it is still difficult to plot its behavior, this new expression is useful for the fact that it enables to compute an estimate for the low temperature regime, since, following the footstep of the previous subsection, the lowest order will be contained in the lowest (Hamming) weight term of the sum, i.e. the one with $i = 1$. We need to compute the term $\sum_{\substack{j\in\{0,1\}^M \\ w(j)=i}} \mathrm{Tr}\Big[\rho_{A_j}\Big]$ for $w(j) = 1$.

Consider the trace of the ancillary density matrix relative to the string of M zeros "**0**":

$$\mathrm{Tr}(\rho_{A_0}) = \sum_{k=0}^{\xi^\star_M-1} \binom{N}{k} P_1^k (1-P_1)^{N-k} + \alpha_{A_0} P_1^{\xi^\star_M} (1-P_1)^{N-\xi^\star_M}, \tag{3.55}$$

where, similarly to the case of $M = 2$, we define

$$\xi_M^\star := \text{argmax}_\xi \left\{ \sum_{k=0}^{\xi-1} \binom{N}{k} \leq 2^{N-M} \right\}, \tag{3.56}$$

$$\alpha_{A_0} := \left\{ 2^{N-M} - \sum_{k=0}^{\xi_M^\star - 1} \binom{N}{k} \right\}. \tag{3.57}$$

Then, for strings with Hamming weight $w = 1$:

$$\begin{aligned} \sum_{\substack{j\in\{0,1\}^M \\ w(j)=1}} \text{Tr}\left[\rho_{A_j}\right] = &\left\{ \binom{N}{\xi_M^\star} - \alpha_{A_0} \right\} P_1^{\xi_M^\star} (1-P_1)^{N-\xi_M^\star} + \\ &+ \sum_{k=\xi_M^\star+1}^{\xi_M'-1} \binom{N}{k} P_1^k (1-P_1)^{N-k} + \\ &+ \left\{ (1+M)\cdot 2^{N-M} - \sum_{k=0}^{\xi_M'-1} \binom{N}{k} \right\} P_1^{\xi_M'} (1-P_1)^{N-\xi_M'} \end{aligned} \tag{3.58}$$

where

$$\xi_M' = \text{argmax}_\xi \left\{ \sum_{k=0}^{\xi-1} \binom{N}{k} \leq 2^{N-M}(1+M) \right\}. \tag{3.59}$$

The lowest order is

$$\sum_{\substack{j\in\{0,1\}^M \\ w(j)=1}} \text{Tr}\left[\rho_{A_j}\right] = \left\{ \binom{N}{\xi_M^\star} - \alpha \right\} P_1^{\xi_M^\star} + \binom{N}{\xi_M^\star + 1} P_1^{\xi_M^\star+1} + O(P_1^{\xi_M^\star+2}). \tag{3.60}$$

At the level of P_1', thus, we are left with

$$P_1'(N,M,P_1) = \frac{1}{M}(C_1(N,M)P_1^{\xi_M^\star} + C_2(N,M)P_1^{\xi_M^\star+1}) + O(P_1^{\xi_M^\star+2}). \tag{3.61}$$

In the low temperature limit $P_1 \simeq e^{-\beta\hbar\omega}$ and $P_1' \simeq e^{-\beta'\hbar\omega}$, giving, at lowest order $\beta\hbar\omega = -\log(C) + l\beta'\hbar\omega$ with $C = C_1$ if $C_1 \neq 0$, and $C = C_2$ otherwise. Taking the low temperature limit is equivalent to taking the limit for $\beta \to \infty$, hence we get, in analogy with the case for $M = 2$:

$$T' \simeq \begin{cases} \dfrac{T}{\xi_M^\star} & \text{if } \binom{N}{\xi_M^\star} \neq \alpha_{A_0}, \\ \dfrac{T}{\xi_M^\star + 1} & \text{otherwise.} \end{cases} \tag{3.62}$$

Notice that, unformally, for $M = N-1$ it is not possible to cool any qubit. Consider $M = N-1$: from the definition $\xi^\star_M = 1$, since

$$\xi'_M = \text{argmax}_\xi \left\{ \sum_{k=0}^{\xi-1} \binom{N}{k} \leq 2 \right\} \tag{3.63}$$

can be solved only by $\xi^\star_M = 1$ for all $M \geq 1$ ($N \geq 2$). Thus,

$$T' \simeq T \quad \text{if} \quad M = N-1. \tag{3.64}$$

An interesting question would be whether this can be proven formally.

3.3.3 Estitmate for $\xi^\star_M$

Equation 3.62 gives an interesting estimate of the final temperature, but as a function of the variable $\xi^\star_M$, whose value depends by N and M. Here we try to obtain an estimate on the value of $\xi^\star_M$, with the final goal of writing an estimate of the temperature with explicit dependence on the parameters N and M.

From the definition

$$\xi^\star_M = \text{argmax}_\xi \left\{ \sum_{0 \leq k < \xi} \binom{N}{k} \leq 2^{N-M} \right\}, \tag{3.65}$$

we notice that the term inside the parentheses represents the cumulative function for the binomial density with probability of single success $p = 1/2$ and N trials:

$$P(X < \xi) = \sum_{0 \leq k < \xi} \binom{N}{k} \frac{1}{2^k} \left(1 - \frac{1}{2}\right)^{N-k} = \frac{1}{2^N} \sum_{0 \leq k < \xi} \binom{N}{k} \tag{3.66}$$

Thus, an equivalent definition is

$$\xi^\star_M := \text{argmax}_\xi \{ P(X < \xi) \leq 2^{-M} \}, \tag{3.67}$$

where $X \sim B(N, \frac{1}{2})$ represents the number of successes for N trials. For large N we can approximate the binomial with the Gaussian distribution:

$$X \sim \mathcal{N}(N/2, \sqrt{N}/2),$$

that is the Gaussian distribution with mean $N/2$ and standard deviation $\sqrt{N}/2$. Moreover we define $Z = 2(X - N/2)/\sqrt{N}$ such that $Z \sim \mathcal{N}(0,1)$. We are left with the problem

$$P(Z < t) = \int_{-\infty}^{t} \frac{e^{-s^2/2}}{\sqrt{2\pi}} ds = \phi(t) \leq \frac{1}{2^M}, \tag{3.68}$$

where $\phi(t)$ is the cumulative function of the Gaussian. To get an explicit relation we need to assume also large M: under this assumption we can approximate $\phi(t) \simeq \frac{e^{-t^2/2}}{|t|\sqrt{2\pi}}$ for $t < 0$, as it corresponds to $\xi^\star_M$, which is always smaller than the mean value. To prove it we iteratively apply integration by parts on the integral

$$\begin{aligned}
\int_{-\infty}^{-|t|} \frac{e^{-s^2/2}}{\sqrt{2\pi}} ds &= \int_{-\infty}^{-|t|} \frac{-s e^{-s^2/2}}{-s\sqrt{2\pi}} ds = \left[\frac{e^{-s^2/2}}{-s\sqrt{2\pi}}\right]_{-\infty}^{-|t|} - \int_{-\infty}^{-|t|} \frac{e^{-s^2/2}}{s^2\sqrt{2\pi}} ds = \\
&= \left[\frac{e^{-s^2/2}}{-s\sqrt{2\pi}}\right]_{-\infty}^{-|t|} + \left[\frac{e^{-s^2/2}}{s^3\sqrt{2\pi}}\right]_{-\infty}^{-|t|} + \int_{-\infty}^{-|t|} \frac{e^{-s^2/2}}{s^4\sqrt{2\pi}} ds = \ldots = \\
&= \frac{e^{-t^2/2}}{\sqrt{2\pi}} \left(\frac{1}{|t|} - \frac{1}{|t|^3} + \frac{3}{|t|^5} + \cdots\right) \\
&\simeq \frac{e^{-t^2/2}}{|t|\sqrt{2\pi}},
\end{aligned} \tag{3.69}$$

where we approximated due to the fact that large M implies large $|t|$, hence we consider the larger term. Then we look for a solution of the identity

$$P(Z < t) = 2^{-M}, \tag{3.70}$$

which explicitly becomes:

$$\frac{e^{-t^2/2}}{|t|\sqrt{2\pi}} = 2^{-M} \Rightarrow \frac{-t^2}{2} - \log(|t|\sqrt{2\pi}) = -M\log(2). \tag{3.71}$$

Again, for large $|t|$, we can neglet the $\log(|t|)$ term:

$$\frac{-t^2}{2} - \log(|t|\sqrt{2\pi}) \simeq \frac{-t^2}{2} = -M\log(2) \Rightarrow t \simeq -\sqrt{2M\log(2)}. \tag{3.72}$$

This is the solution for the quantile of the variable Z, for X we have to consider $\xi = \frac{N}{2} + \frac{\sqrt{N}}{2} t$, leading to:

$$\xi \simeq \frac{N}{2} - \frac{\sqrt{N}}{2}\sqrt{2M\log(2)}. \tag{3.73}$$

At this point, we can plug this estimate in the low temperature limit:

$$T' \simeq \frac{2T}{N - \sqrt{2NM \log 2}}, \tag{3.74}$$

where the possible coefficient +1 in the denominator is neglected in the limit for high N with finite M. This equation connects the initial number of qubits N at temperature T with the final number of qubits M at temperature T', providing a practical estimate of the amount of cooling achievable on a quantum system. However, note that, due to the assumptions taken, this does not hold for small M or for $M \simeq N$: for the general estimate, one should refer to Equation 3.62.

Conclusions

In this work, we have addressed the idea of cooling multiple qubits using a single global unitary operation $\mathscr{U}$.
After an in-depth introduction to the main players that were necessary to mathematically formulate the problem, focused on recalling the main ideas of Quantum Thermodynamics and Quantum Computing, we exploited the idea of cooling a quantum system through a quantum algorithm. This was done by taking a historical approach, starting by mentioning the first works, where the aim was to solve the problem of initialization in NMR quantum computation. Towards the same goal, cooling algorithms coupled at rounds with an exernal bath (heat bath algorithmic cooling) were introduced. Then, we argued that the recent introduction of new platforms for quantum computation with lower starting temperatures led to a complete re-evaluation of closed dynamics cooling. This naturally led us to the central reference of our work: we have introduced the general idea behind the paper published by Oftelie, De Pasquale, and Campisi [21] and re-derived their main results. At the same time, we introduced a slight variation of the previous problem, as offered by [22]: here, initial qubits were considered with generic temperature, in principle different from each other, and general results on the eigenvalues-swapping procedure were obtained.

Armed with this theoretical background, we were able to correctly formulate the initial problem. We initially focused on the implication of requiring a unique final temperature for a multiple number of qubits, obtaining highly non-trivial results on the feasibility of this operation.
The first crucial result involves a necessary condition that must have to be fulfilled to guarantee the possibility of having a final target state with a unique temperature. This is composed by a set of identities that the probabilities of the target system should obey, expressed as the trace of an ancillary density matrix. The structure shows the strictly precise configuration that a general unitary operator should lead to and, also, translates the problem of minimizing the temperature of M qubits into an highly symmetric problem. Then, we focused on

the mathematical structure hidden within the unique temperature condition, and we showed that it formally corresponds to a binomial-partitioning problem, where two binomial structures made of total "boxes" (or trials, based on the perspective from which one thinks about the binomial) N and M are asked to "fit" into each other. It is fascinating to see that this is unexpectedly frequent for small values of M, giving a potential technological solution for cooling with few resources (for example, by using 10 initial qubits, we can cool 4 of them at the same temperature). Then, we evaluated possible directions for when the numbers N, M do not present a solution to the partition problem. We realized that by applying a Quantum Fourier Transform on the right subspaces, we can recover a final configuration that presents a unique temperature within the M target qubits, at the cost of introducing off diagonal terms.

The last conclusive result regards the amount of cooling that we can reach. In the low temperature regime, easily reached by modern quantum computers, we found an estimate on the cooling that such a framework would be able to provide, with a compact formula that links the final temperature of the target qubits T', with the initial temperature T and to the coefficient $\xi^{\star}_{M}$. This depends on N and M and for it we provide an explicit estimate as a function of these numbers.

This work naturally opens several directions for future research. In the first place, a proper analysis of the general scenario with qubits that are initially at different temperatures can be studied, where the M target qubits can be required to be identical or not. General bounds on the final temperature reached for identical final target qubit would be of particular interest for technological applications. On the other side, the task of cooling can also be studied with different initial configurations, by considering qubits that present correlations, both classical and quantum.

In the present work, we did not address the problem of minimal work required, nor of computational complexity, and are both directions that can lead to further considerations. In particular, it would be interesting to see if an algorithmic version of Mpemba effect could be proven in the framework of Dynamic Cooling.
Overall, the relative youth of this field of research enables the exploration of a huge variety of different scenarios that can play a role in technological innovation and in deepening our understanding of reality at the quantum scale.

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