Achievable Polarization for Heat-Bath Algorithmic Cooling

by

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Autor’s declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

Highly pure quantum states play a central role in applications of quantum information science, both as initial states for quantum algorithms and as resources for quantum error correction. Controlled preparation of pure enough quantum states that satisfy the threshold for quantum error correction remains a challenge, not only for ensemble implementations like nuclear magnetic resonance (NMR) or electron spin resonance (ESR) but also for other technologies. Heat-bath algorithmic cooling (HBAC) is a promising method to increase the purity of a set of qubits coupled to a bath. In this thesis, we investigated the achievable polarization of this technique by analyzing the limit when no more entropy can be extracted from the system. In particular, we give an analytic form of the maximum polarization achievable for the case when the initial state is totally mixed, and the corresponding steady state of the whole system. Furthermore, we give the number of steps needed to get a specific required polarization (the exact number for the two qubit case and an upper bound for more general cases).

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Especially, I would like to thank my supervisor Dr. Raymond Laflamme for the great help and support that I have received from him. He has been exceptionally generous with his time and support over the past two years. I have been very lucky to have a fantastic supervisor.

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Dedication

To my parents.
I have learnt the values of determination
and hard work by watching them.

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Chapter 1

Introduction

Quantum information processing brings novel techniques for cooling physical systems by manipulating entropy at the quantum level [2–6]. Understanding this kind of processes and their cooling limits is fundamental from both theoretical and experimental points of view. This can help us to study quantum thermodynamics properties and to discover features of physics at low-energy states. Furthermore, these methods have extremely important applications in quantum information science. They constitute a potential solution to purify quantum systems in ensemble implementations [7–13], which is one of the major challenges in quantum computing.

1.1 Purification of qubits for quantum computing

1.1.1 Quantum computers

Quantum computing exploits the laws of quantum mechanics to process information in ways that would be impossible by classical computers. Quantum phenomena, such as quantum superposition and entanglement, enable the development of efficient algorithms that considerably outperform any known classical algorithm. Two of the most important examples are factoring large numbers [14] and simulating quantum systems. It promises the possibility of dramatic speed up of computations and simulations.

The physical construction of a quantum computer faces serious challenges. There is a set of basic criteria required for the implementation of such a device. The most widely accepted criteria is given by DiVincenzo, which consists of 5 requirements [15]:

1. Well characterized qubits

2. The ability to initialize qubits to a pure state.

3. Long relevant decoherence times much longer than the gate operation time

4. A universal set of quantum gates

5. A qubit-specific measurement capacity

In this work, we focus on the second requirement, the preparation of highly pure states.

1.1.2 State-Preparation

Controlled preparation of pure enough quantum states is at the core of the practical applications of quantum information science, from the initialization phase of most quantum algorithms to the need for a reliable supply of ancilla qubits in quantum error correction.

Finding a scalable way to reach approximate pure states constitutes a challenge in many different quantum computing experimental implementations, especially the ones that rely on an ensemble of qubits, such asnuclear magnetic resonance (NMR) or electron spin resonance (ESR) [16]. In some technologies, highly pure states can be achieved through projective measurements, but in measurement of ensembles such luxury is not possible. In ensemble implementations, identical copies of a quantum system are manipulated in parallel, and only expectation values of certain observables are measurable. This restriction, with the fact that in typical ensemble systems the qubits are highly mixed at room temperature, constitutes an extremely difficult problem.

1.1.3 Heat-Bath Algorithmic Cooling

A potential solution is algorithmic cooling (AC), a protocol based on information theory ideas, which is designed to purify a set of qubits by removing entropy of a subset of them at the expense of increasing the entropy of others [17, 18]. An explicit way to implement this protocol in ensemble quantum computers was given by Schulman et al. [19]. They showed that it is possible to reach polarization of order unity using only a number of qubits that scale polynomially as a function of the initial polarization. This scheme was improved by adding contact with a heat-bath, used to extract entropy from the system [2], a process known as heat-bath algorithmic cooling (HBAC). Based on this work, many cooling algorithms have been designed [4–6, 20–23]. HBAC is not only of theoretical interest, experiments have already demonstrated an improvement in polarization using this protocol with a few qubits [7–13], where a few rounds of HBAC were implemented.

Through numerical simulations, Moussa [20] and Schulman et al. [5] observed that if the polarization of the bath (ϵ_b) is much smaller than 2^{-n}, where n is the total number of qubits, the asymptotic polarization reached will be $\sim 2^{n-2}\epsilon_b$. However, when ϵ_b is greater than 2^{-n}, a polarization of order one can be reached.

1.2 Goal and results

Even though HBAC has been already demonstrated in the lab and has been studied through numerical simulations, the cooling limits of these techniques were not completely well understood. The problem of finding the maximum achievable polarization for a number of qubits n remained open for the past decade. The purpose of this master project is to study the physical cooling limits of HBAC, and how they can be used to improve state preparation techniques in experimental implementations.

We investigated the achievable polarization for the case of cooling a qubit using a general spin l (or n' qubits, which is a special case of this, for $2l+1 = 2^{n'}$), and m extra qubits that get contact with a bath.

The main result of this thesis (see chapter 4) is the analytic expression for the asymptotic polarization as a function of the number of qubits and as a function of the heat-bath polarization.

We first present the cooling limit conditions; and from this, we find the steady state for maximally mixed initial states. Our exact expression reproduce the numerical results, and improve the previous upper bound found by Schulman et al. [5, 6, 20]. We showed that the asymptotic polarization goes to 1 doubly exponentially in the number of qubits (or exponential as a function of the size of the Hilbert space of the system). Finally, with our analysis it becomes easy to find the number of compression/cooling rounds required to achieve a certain amount of polarization (we have the exact number for the three qubits case and an upper bound for more general cases).

Our all original contributions are presented in chapter 4, 5 and 6. The results of this work have been accepted for publication in Physical Review Letters [1]).

Chapter 2

Background

In this chapter, we provide the background needed to understand the problem of preparing highly pure states in ensemble implementations. We also show how energy transport and information processing are two sides of the same coin. In fact, quantum information theory can provide new interesting ways to cool physical systems by manipulating information at the quantum level [2–6]. These schemes can reach lower temperatures than the ones obtained by conventional methods in the laboratory.

2.1 Polarization and temperature of an ensemble of qubits

Consider an ensemble of qubits, i.e. a collection of independent, identical two-level quantum systems. Let $|0\rangle$ and $|1\rangle$ be the two levels, with corresponding energy eigenvalues E_0 and E_1. When the system is left undisturbed for a long time, in contact with the molecular surroundings, it reaches a state of thermal equilibrium with that environment. In thermal equilibrium at temperature *T*, the following properties hold [24]:

1. The probability of occupancy of a given energy level $|i\rangle$ is given by the Gibbs distribution, $n_{E_i}(E_i) = \exp[-E_i/kT]/Z$, where Z is the partition function ($Z = \exp[-E_0/kT] + \exp[-E_1/kT]$).

2. The coherences between the states are all zero.

Accordingly, the average-density matrix over all members of the ensemble can be written as follows:

$$\rho^{eq} = \begin{pmatrix} n(E_0) & 0 \\ 0 & n(E_1) \end{pmatrix} = \frac{1}{Z} \begin{pmatrix} \exp[-E_0/kT] & 0 \\ 0 & \exp[-E_1/kT] \end{pmatrix}. \tag{2.1}$$

This density matrix is used to represent the state of any qubit of the ensemble in thermal equilibrium [24]. In ensemble implementations only expectation values are measurable, there is no access to individual qubits. Moreover, in most cases the state of the system is highly mixed.

The ***polarization***, also called the *bias*, ϵ_b, is defined as the excess population in the energetically-favorable $|0\rangle$ state,

$$\epsilon_b = n\left(E_0\right) - n\left(E_1\right) = \frac{e^{-E_0/kT} - e^{-E_1/kT}}{e^{-E_0/kT} + e^{-E_1/kT}}, \tag{2.2}$$

$$\epsilon_b = \tanh\left(\frac{E_0 - E_1}{2kT}\right) \equiv \tanh\left(\epsilon\right), \tag{2.3}$$

where $\epsilon \equiv \frac{E_\delta}{kT}$, and E_δ is the energy splitting between the two levels, $E_\delta = \left(E_0 - E_1\right)/2$. From eq.(2.3), cooling the system and increasing its polarization are closely related, especially for a fixed energy gap (E_δ). The absolute value of the polarization, $|\epsilon_b|$, ranges from 0 to 1. In the limit when the temperature is zero, the polarization is 1.

Then, the density matrix describing the state of qubit of the ensemble in the thermal equilibrium can be written, in terms of polarization, as follows:

$$\rho_{\epsilon_b} = \frac{1}{2}\begin{pmatrix} 1+\epsilon_b & 0 \\ 0 & 1-\epsilon_b \end{pmatrix}. \tag{2.4}$$

Some authors, such as Schulman et al. [5, 6], use $\epsilon = \operatorname{arctanh}\left(\epsilon_b\right)$ as polarization. The corresponding density matrix of eq.(2.4) in terms of ϵ is

$$\rho_{\epsilon_b} = \frac{1}{e^{-\epsilon} + e^{\epsilon}}\begin{pmatrix} e^{\epsilon} & 0 \\ 0 & e^{-\epsilon} \end{pmatrix}. \tag{2.5}$$

Note that using this definition also gives the fact that decreasing temperature is the same that increasing polarization (and conversely) for a fixed energy gap (E_δ). Both definitions, ϵ_b and ϵ, are very close to each other for small energy gap and high temperature, $\epsilon_b \approx \epsilon$. However, they differ considerably for low temperatures and big energy gap. The polarization defined as ϵ goes to infinity when temperature goes to zero.

2.1.1 Ensemble of qubits in NMR

In the context of NMR quantum information processing [25, 26], the ensemble consists of a bulk sample of identical molecules, each with n distinguishable nuclear spins. Each molecule is considered as an individual n-qubit processor.

The interaction of a spin-$\frac{1}{2}$ with an external static magnetic field, gives the two eigenstates required for a qubit. The energy splitting, Zeeman splitting, between those two levels is proportional to the field strength, B, and is much smaller than thermal energy, kT, at room temperature, where k is the Bolztmann constant. The corresponding polarization, calculated using eq.(2.3), is

$$\epsilon_b \approx \frac{\mu B}{2kT} \approx \epsilon, \tag{2.6}$$

where μ is the magnetic moment of the spin in question. For the case of larger spin, l, the analysis is similar [24].

For protons at room temperature, in a $B = 7T$ field, the polarization is of the order of magnitud of 10^{-5}. It has been shown that even with such a low polarization, it is possible to get computational advantages over classical computation in some cases (for example, for simulating some physical systems [27], measuring the average fidelity decay [28], among others). However, for general purposes of quantum computing, purification remains necessary [29].

Different techniques have been implemented to boost the polarization of the nuclear spins in NMR to solve the initialization problem. Most of these methods are based on pseudo-pure state (PPS) preparation techniques [30, 31], nevertheless these procedures have an exponential loss of signal-to-noise with the number of qubits [2]. It is still conceivable that in conjunction with other methods, the PPS techniques would play a role in initializing scalable ensemble quantum computing. Therefore, finding ways to produce highly polarized states (or at least with a polarization level where it would be feasible to use PPS) remains indispensable.

2.2 Entropy and Purity

In quantum information theory, the Von Neumann entropy for a quantum system with state ρ is defined as $S(\rho) \equiv -\mathrm{tr}(\rho \log_2 \rho)$. For a diagonal density matrix, that expression is reduced to the Shannon entropy of the probability distribution given by the diagonal entries of ρ. Then, this can be written as $S(\rho) = -\sum_x \lambda_x \log \lambda_x$, where λ_x are the eigenvalues of the diagonal density matrix ρ.

The level of purity of a system with quantum state ρ is commonly measured as $Purity := \mathrm{Tr}\,(\rho^2)$. The purity goes from $\frac{1}{d}$ to 1, i.e. from maximally mixed state to pure state, for states of dimension d. ρ is a pure state if and only if $\mathrm{Tr}\,(\rho^2) = 1$.

The entropy gives a measurement of the mixedness of a state. Entropy equal to 0 corresponds to the case when state of the qubit is perfectly known, i.e. a pure state.

For an ensemble of qubits with polarization ϵ_b, the state of each quibit can be considered as the one given by (2.4), its entropy has the following form:

$$S(\rho_{\epsilon_b}) = -\frac{1+\epsilon_b}{2}\log_2\left(\frac{1+\epsilon_b}{2}\right) - \frac{1-\epsilon_b}{2}\log_2\left(\frac{1-\epsilon_b}{2}\right), \tag{2.7}$$

and the corresponding purity evaluates to

$$Purity = \mathrm{Tr}\left(\rho^2\right) = \frac{1}{2}\left(1+\epsilon_b^2\right). \tag{2.8}$$

Fig.(2.1) shows the entropy and purity as a function of the polarization of the system. Having high polarization corresponds to having high purity and low entropy.

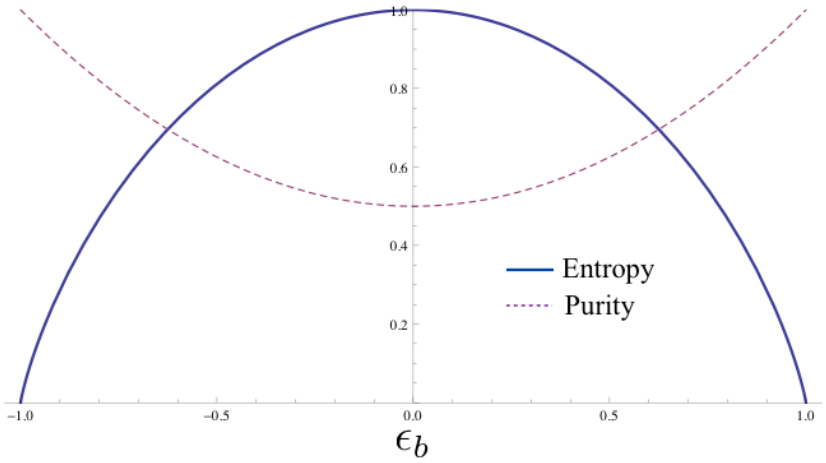

Figure 2.1: Entropy and purity of a single qubit as a function of the polarization are shown in solid-blue line and dashed-pink line, respectively. This illustrates the mapping described between the polarization, entropy and purity.

2.3 Cooling Methods

The introduced concepts establish a close interrelationship between increasing the polarization, lowering the temperature, decreasing the entropy, and purifying the system. From this, it is possible to plan different strategies to purify the qubits in ensemble implementations.

The equation of the polarization, $\epsilon_b = \tanh\left(E_\delta/kT\right)$, suggests two obvious methods to purify the system. The first one is to directly cool the system, i.e. decreasing the temperature of the system and environment. However, in general this is experimentally hard, considering that the temperature should be extremely low to obtain high enough polarization. The second approach

is to increase the energy gap E_δ, but this approach is technological dependent; for example, in NMR, that would mean increasing the magnetic field (eq.(2.6)); nevertheless, to increase the magnetic field, at least one order of magnitude, from the typical current values would require a big technological advancement.

More interesting strategies are obtained if we think in the redistribution of the internal entropy over all the qubits in the system, which could be possible using the tools of quantum information processing. This kind of methods are called algorithmic cooling techniques. Remarkably, these procedures are not technological dependent [2–6], as it is explained in the next section and next chapter.

2.3.1 Algorithmic Cooling

An internal redistribution of the entropy over all the qubits in the system can be obtained through quantum logic operations to get a subset of highly-polarized qubits from an initial set of weakly-polarized ones [2–6]. This carries out a reversible entropy compression process in which the system results in a separation of cold and hot regions. Schulman and Vazirani [3], presented an explicit cooling method which recursively applies majority gates, inspired by the Von Neumann's ideas of the extraction of fair coin flips from a sequence of biased ones. Their algorithm cooling method allows purify $\frac{1}{20}\epsilon^2 n$ qubits to a bias of $1 - 2n^{-10}$, from an initial set of n qubits with polarization ϵ. They proved that the optimal adiabatic compression is achieved with this algorithm; however, it is impractical with current technology. For room temperature biases ($\epsilon_b \approx 10^{-5}$), approximately $2\text{x}10^{12}$ qubits are required to boost the polarization close to 1. The cooling limits of this method are imposed by the bound Shannon entropy and the preservation of the eigenvalues.

In 2002, Boykin et al.[2] improved the AC idea by adding contact with a heat-bath of partially polarized qubits, with the goal of pumping entropy out of the original system and sent it into the heat-bath. This kind of methods are called heat-bath algorithmic cooling, and they can transcend the previously mentioned shortcomings, as explained in the next section in more detail.

Based on this work, many cooling algorithms have been designed and tested experimentally [4–6, 20–22]. HBAC is not only of theoretical interest, experiments have already demonstrated an improvement in polarization using this protocol with a few qubits [7–13], where a few rounds of HBAC were implemented; and a more realistic implementation has been studied in the paper [23].

Chapter 3

Heat Bath Algorithmic Cooling

Heat-bath algorithmic cooling (HBAC) purifies qubits by applying alternating rounds of entropy compression and pumping entropy into a thermal bath of partially polarized qubits. These steps are explained in detail in this chapter.

The system consists of a string of qubits: one qubit (spin$-1/2$, also called the target qubit) which is going to be cooled; one qudit (called the scratch system, which can be a spin$-l$ or a string of qubits) which aids in the entropy compression; and m reset qubits that can be brought into thermal contact with a heat-bath of polarization ϵ_b. Having the spin$-l$ is equivalent to having n' qubits if the dimension of their Hilbert spaces is the same, i.e. if $d = 2l + 1 = 2^{n'}$. We will also refer to the target qubit and the scratch qudit as the computational qubits (Fig. 3.1).

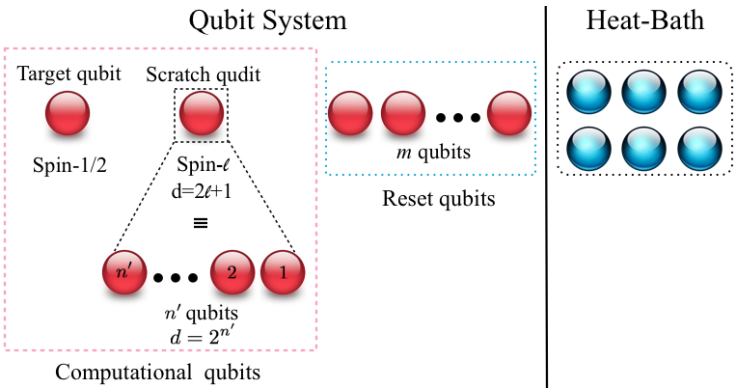

Figure 3.1: HBAC can cool the target qubit by compressing entropy into m reset qubits and a $d-$dimensional spin$-l$ (or a string qubits of Hilbert space of dimension d); then, HBAC pumps entropy from the qubit system into a heat-bath by refreshing the m reset qubits.

The idea of HBAC is to first re-distribute the entropy among the string of qubits by applying an entropy compression operation U. This is a reversible unitary process that extracts entropy

from the computational qubits as much as possible and concentrates entropy in the reset qubits of the system. This process results in the cooling of the computational qubits while warming the reset qubits (Fig. 3.2).

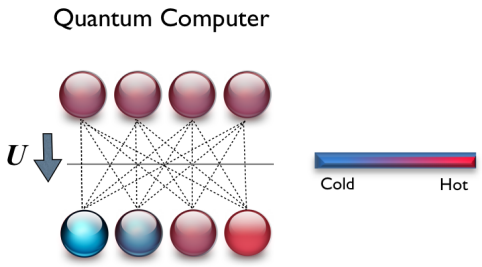

Figure 3.2: Entropy compression step. A compression operation U pushes the entropy into one side of the system. In the figure, the top part represents the string of qubits before the compression. Dotted lines indicate re-distribution of entropy among all qubits, resulting in the separation of cold and hot regions as shown in the bottom part.

The second step is to refresh the system using the heat-bath for removing entropy. The heat-bath is assumed to have infinite heat capacity, such that the action of qubit-bath interaction on the bath is negligible. There are different ways to couple a quantum system with a bath to extract entropy from the system. One example is the rethermalization of the reset qubits to the heatbath temperature, which is equivalent to swapping the reset qubits with qubits of the heat-bath. This particular refresh procedure is used in the PPA method, as explained in the next section (Fig. 3.3).

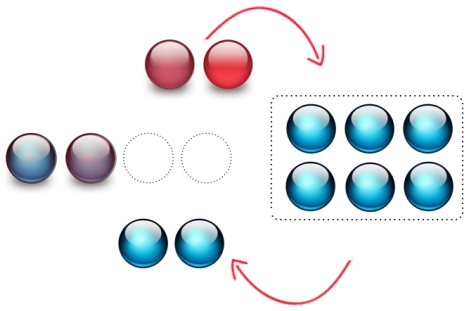

Figure 3.3: Example of refresh step, used in the PPA method. The reset qubits are brought into thermal contact with a heat-bath to pump entropy out from the qubit system. In the figure, two reset qubits are used as an example.

These reversible compression and refreshing steps are iteratively applied until the target qubit reaches the desired temperature or until the cooling limit is reached.

The physical requirements for computational and reset qubits are different. A computational

qubit should have long relaxation time to remain polarized after being cooled through entropy compression, and a reset qubit should strongly interact with the bath in order to rapidly relax and attain the bath temperature.

3.1 The Partner Pairing Algorithm (the PPA) method

For our study, we used a HBAC algorithm called the Partner Pairing Algorithm (PPA), which was invented by Schulman et al.[5]. This protocol gives the optimal physical cooling in terms of entropy extraction, under the assumption that the refresh step re-thermalizes the reset qubits to the heat-bath temperature [5, 6].

In the PPA, the entropy compression operation, U, makes a descending sort of the diagonal elements of the system's density matrix. I.e., this step rearranges the eigenvalues such that states in increasing lexicographic order have non-increasing probability. Therefore, the probability amplitude of states starting with 0 (000, 001, etc.) will take the biggest values of the diagonal elements, while that of states starting with 1 will take the smallest ones. This operation aims to increase the polarization of the first qubit. The compression can no longer improve the polarization of the first qubit once the states are already ordered as described above. In this step,

$$\rho \xrightarrow{Compression} \rho' = U\rho U^{\dagger}. \tag{3.1}$$

The particular computations required in this step vary in a complex way, since they depend on the number of qubits, the heat-bath polarization, and the polarization of each qubit of the system at that moment.

In the refresh step, the m reset qubits are brought into thermal contact with the bath to be refreshed. This step is equivalent to tracing-over the reset qubits, and replacing them with qubits from the heat-bath, cooling the qubit system (see Fig. 3.3). This means that the maximum polarization that the reset qubit are able to obtain in this step is equal to the polarization of the heat-bath, ϵ_b. We also assume that the heat-bath has large heat capacity and that the action of qubit-bath interaction on the bath temperature is negligible. In this step, the system's density matrix changes as follows:

$$\rho' \xrightarrow{Refresh} \rho'' = \mathrm{Tr}_{m_{qubits}}\left(\rho'\right) \otimes \rho_{\epsilon_b}^{\otimes m}. \tag{3.2}$$

where $\rho_{\epsilon_b} = \frac{1}{2}\begin{pmatrix} 1+\epsilon_b & 0 \\ 0 & 1-\epsilon_b \end{pmatrix}$ is the state of a qubit from the bath, and ϵ_b is the heat-bath polarization (some authors, such as Schulman et al. [6], use $\epsilon = \mathrm{arctanh}\epsilon_b$ as polarization).

The total effect of applying these two steps, an iteration of the PPA method, on a system with state ρ can be expressed as follows:

$$\rho \to \rho'' = \mathrm{Tr}_{m_{qubits}} \left(U \rho U^{\dagger} \right) \otimes \rho_{\epsilon_b}^{\otimes m} \tag{3.3}$$

3.1.1 Illustrative example: PPA for three qubits

In order to illustrate how the PPA method works, here it is applied on a particular system of three qubits (one reset qubit and two computational qubits). Consider the 3-qubit system initially in a totally mixed state, ρ_0, and the qubits of the heat-bath in a state with polarization ϵ_b.

First iteration

First, contact between the reset qubit and the heat-bath is established. Then the compression operator U permutes the probabilities of the basis states and sorts them in non-increasing order, as follows:

$$\mathrm{d}(\rho_0) = \frac{1}{8}\begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix} \xrightarrow{R} \mathrm{d}(\rho_0') = \frac{1}{8}\begin{bmatrix}1+\epsilon_b\\1-\epsilon_b\\1+\epsilon_b\\1-\epsilon_b\\1+\epsilon_b\\1-\epsilon_b\\1+\epsilon_b\\1-\epsilon_b\end{bmatrix} \xrightarrow{C} \mathrm{d}(\rho_0'') = \frac{1}{8}\begin{bmatrix}1+\epsilon_b\\1+\epsilon_b\\1+\epsilon_b\\1+\epsilon_b\\1-\epsilon_b\\1-\epsilon_b\\1-\epsilon_b\\1-\epsilon_b\end{bmatrix}, \tag{3.4}$$

where $\mathrm{d}(\rho)$ are the eigenvalues of ρ, and R and C stand for refresh and compression steps, respectively. This compression is equivalent to swapping the first computational qubit with the reset qubit. After this iteration, the polarization of the first qubit is increased from 0 to ϵ_b.

Analyzing the entries of $\mathrm{d}(\rho_0')$, it is possible to know which permutations are required in order to have states with non-increasing probabilities in the lexicographic order. For this specific case, the entropy compression operation should swap the states $\{|001\rangle, |011\rangle\}$ for the states $\{|100\rangle, |110\rangle\}$. This transformation can be performed by applying the unitary matrix shown in Fig. 3.4, to obtain the desired state $\mathrm{d}\left(\rho_1\right) := \mathrm{d}\left(\rho_0''\right)$.

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} =$$

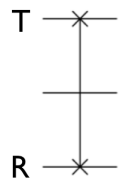

Figure 3.4: Matrix and circuit symbol representing the unitary operation of the first iteration of the PPA on three qubits that are initially in a completely mixed state. In the circuit diagram, the top qubit is the target qubit (denoted T) and the bottom qubit is the reset qubit (denoted R). In the first iteration, the compression gate swaps the target qubit and the reset qubit.

Second iteration

Upon repeating above two steps again, we effectively swap the second computational qubit with the reset qubit that is at thermal equilibrium with the bath, as follows:

$$\mathrm{d}(\rho_1) := \mathrm{d}(\rho_0'') \xrightarrow{R} \mathrm{d}(\rho_1') = \frac{1}{8}\begin{bmatrix} (1+\epsilon_b)^2 \\ 1-\epsilon_b^2 \\ (1+\epsilon_b)^2 \\ 1-\epsilon_b^2 \\ 1-\epsilon_b^2 \\ (1-\epsilon_b)^2 \\ 1-\epsilon_b^2 \\ (1-\epsilon_b)^2 \end{bmatrix} \xrightarrow{C} \mathrm{d}(\rho_1'') = \frac{1}{8}\begin{bmatrix} (1+\epsilon_b)^2 \\ (1+\epsilon_b)^2 \\ 1-\epsilon_b^2 \\ 1-\epsilon_b^2 \\ 1-\epsilon_b^2 \\ 1-\epsilon_b^2 \\ (1-\epsilon_b)^2 \\ (1-\epsilon_b)^2 \end{bmatrix}. \tag{3.5}$$

The entropy compression operation is performed by applying the unitary matrix shown in Fig. 3.5.

$$\begin{bmatrix} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{bmatrix} \equiv$$

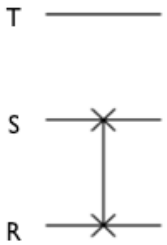

Figure 3.5: Matrix and circuit symbol representing the unitary operation of the second iteration of the PPA on three qubits that are initially in a completely mixed state. In this iteration, the second qubit and the reset qubit are swapped.

In this iteration, the polarization of the first computational qubit remains the same, while the polarization of the second qubit is increased from 0 to ϵ_b .

Third iteration

If the refresh and compression steps are repeated once more,

$$\mathrm{d}(\rho_2) := \mathrm{d}(\rho_1'') \xrightarrow{R} \mathrm{d}(\rho_2') = \frac{1}{8}\begin{bmatrix} (1+\epsilon_b)^3 \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1-\epsilon_b)^3 \end{bmatrix} \xrightarrow{C} \mathrm{d}(\rho_2'') = \frac{1}{8}\begin{bmatrix} (1+\epsilon_b)^3 \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)^2(1-\epsilon_b) \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1+\epsilon_b)(1-\epsilon_b)^2 \\ (1-\epsilon_b)^3 \end{bmatrix}. \quad (3.6)$$

In this iteration, the polarization of the first qubit increases to $1.5\epsilon_b - 0.5\epsilon_b^3$.

$$\begin{bmatrix} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{bmatrix} \equiv$$

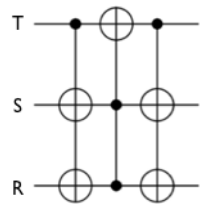

Figure 3.6: Matrix and circuit symbol representing the unitary operation of the third iteration of the PPA on three qubits that are initially in a completely mixed state. This iteration boosts the first qubit polarization to $1.5\epsilon_b - 0.5\epsilon_b^3$. From the second round of HBAC and on, entropy compressions are the repetition of the second and third iterations.

In the next steps, the required compression gates are alternating applications of the operations corresponding to second and third iterations.

The evolution of the polarization of the first qubit under the PPA with is $\epsilon_b << 1$ shown in Fig. 3.7. The circuit asymptotically boosts the polarization on the first qubit up to twice the heat-bath polarization; this limit is discussed in the next section.

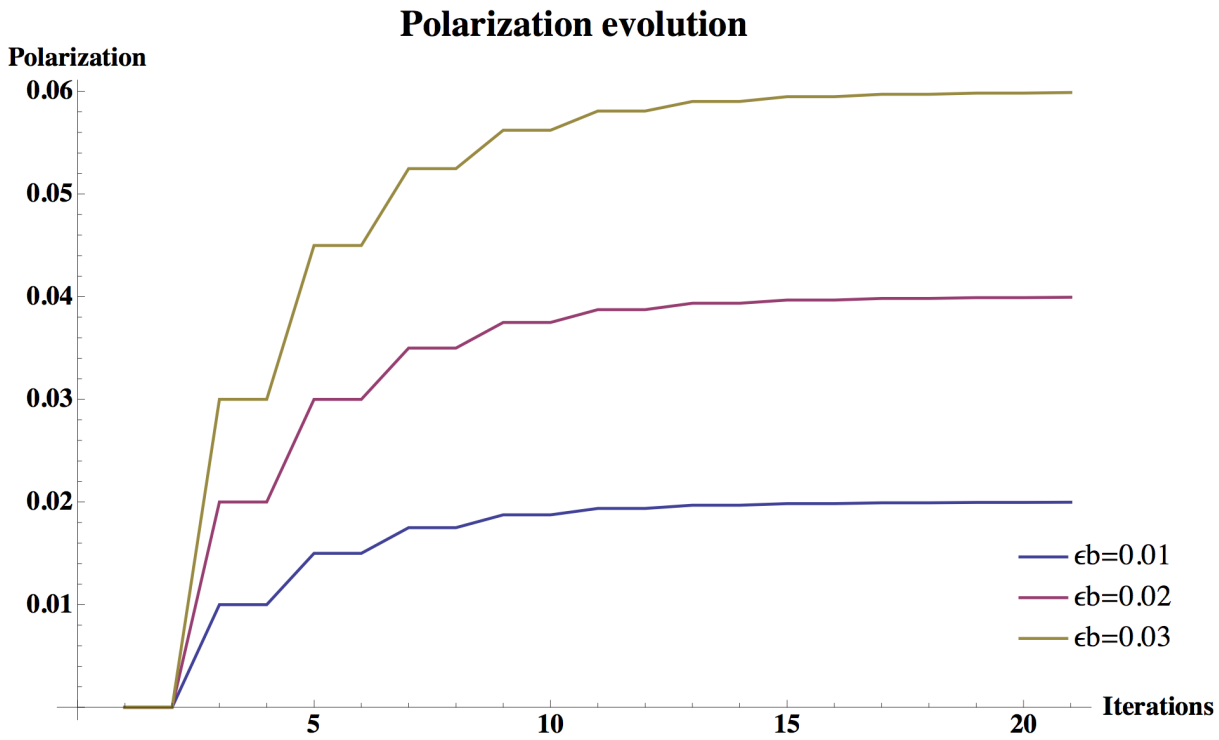

Figure 3.7: Evolution of the target qubit polarization under the PPA method, using a system of 3 qubits, for three values of heat-bath polarization ϵ_b. Each iteration consists of a reset and a compression procedure. Note the asymptotic polarization is $2\epsilon_b$, as expected for $\epsilon_b << 1/2$ in the case of three qubits.

The quantum circuit required to perform the PPA on the three qubits, initially in the totally mixed state, is showed in the Figure 3.8, just for first five iterations (subsequent iterations are just the repetition of the second and third iteration).

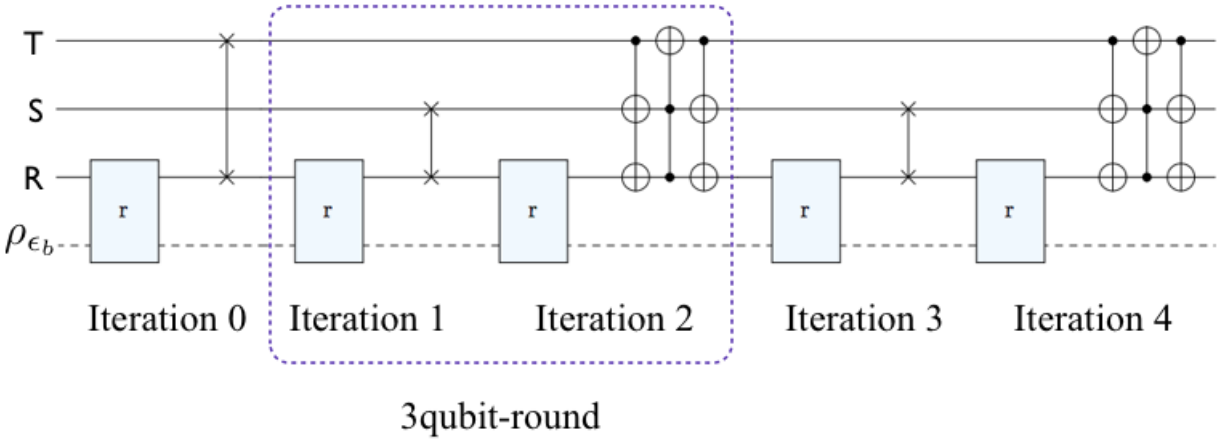

Figure 3.8: Quantum circuit for the PPA method on a system of three qubits starting in total mixed state. In the circuit diagram, the target, the scratch and the reset qubits are denoted T, S, and R, respectively; the dashed line corresponds to the heat-bath and r stands for the refresh operation. The figure shows only the first five iterations of the circuit (an iteration consists of one refresh step plus one compression step), subsequent iterations are just the repetition of the iterations 1 and 2 (a 3qubit-round).

3.2 Experimental implementation of HBAC

Experiments have already demonstrated an improvement in polarization using HBAC with a few qubits [7–13, 32], where a few rounds of HBAC were achieved. It was successfully implemented in liquid state NMR [7–10], solid state NMR [11, 12], quantum optics [33], and ion traps [34]. Furthermore, the possibility to implement HBAC using electron spin resonance (ESR) at high polarization is currently being studied [13].

In the next subsection, we present a short review of HBAC experiments in liquid state NMR, in solid state NMR and in ESR.

3.2.1 Experimental HBAC with NMR and ESR

Experimental realization of algorithmic cooling requires high fidelity control and the ability to reset qubits. Liquid State NMR Quantum Information Processing (LSNMR QIP) has successfully demonstrated precise quantum control up to 12 qubits; however, it presents difficulties to refresh qubits. The only way to reset qubits relies on spin-lattice relaxation, characterized by the time scale of relaxation time T1. Reset qubits must have very short T1 to rapidly relax and attain the bath temperature. This short T1 on the reset qubit limits its T2 and the fidelity of control. Despite these limitations, the first preliminary steps towards full PPA was experimentally

realized in LSNMR by using protons (^{1}H nuclei) as reset qubits and ^{13}C nuclei as computational qubits [9, 32]. These experiments showed selective reset operations to polarize all three spin qubits close to the bath temperature. Nevertheless, the compression step which polarizes a target qubit colder than the heat bath was not implemented. Meanwhile, Chang et al. implemented cooling solely by the final compression gate on three fluorines in C_2F_3BR using LSNMR. Full implementation of HBAC in LSNMR was accomplished much later in [35].

On the other hand, Solid State NMR (SSNMR) offers a reset step that does not require a relaxation process in the system of interest by using a network of dipolar coupled spins as a spin bath. The decoherence rates can be made slow using refocusing techniques, while spin-spin couplings, which are much larger than in LSNMR, can be exploited to realize faster quantum gates [25]. Moreover, SSNMR experiments can be operated at low temperature, providing a higher bath polarization than LSNMR. The first experimental demonstration of HBAC using SSNMR was done by Baugh et al. in 2005 [11]. They implemented the PPA for three qubits using a single crystal of malonic acid $CH_2(COOH)_2$ as quantum processor at $B_0 = 7.1T$ and room temperature. In 2008, Ryan et al. experimentally demonstrated nine iterations of algorithmic cooling in the same experimental system (malonic acid) [12]. They achieved a polarization in the target qubit of $1.69\epsilon_b$, while the corresponding theoretically polarization is $1.94\epsilon_b$. Here, the experimental error was dominated by two factors, the imperfection of ^{1}H decoupling and a non-ideal process of spin diffusion in the network of dipolar coupled protons in the bath.

The fundamentals of electron spin resonance (ESR) quantum computing are analogous to NMR quantum computing, and many of the techniques used for manipulating nuclear spins can also be applied to control electrons. The combination of electron and nuclear spin resonance in hyperfine-coupled quantum processors can provide more advantages. One obvious advantage is that higher gyromagnetic ratio of an electron γ_e (about 660 times greater than that of proton) leads to higher polarization. Decoherence and relaxation rates also scale with γ and hence electron T1 relaxation rate is about 3 orders of magnitude larger than that of nuclei. Thus, the electron spin is an excellent candidate for the reset qubit, which can be refreshed simply by waiting for a time about 5T1. The anisotropic hyperfine interaction gives an advantage for designing nuclear quantum gates, since it provides a control handle for fast manipulations of nuclear spins. But, on the other hand, if the anisotropic hyperfine interaction is strong, it could represent a problem, since the electron T1 relaxation process induces nuclear polarization decay in the presence of anisotropic hyperfine interaction. Fortunately, one can choose the crystal orientation to reduce the anisotropic hyperfine coupling strength so that the nuclear spin decay induced by electron T1 is small enough to allow cooling of a target spin below bath temperature. The control universality of an electron and a nuclear spin coupled system via anisotropic hyperfine interaction was proved in [36], and demonstrated experimentally in [37] for a single nuclear spin qubit gate and in [38]

for a gate involving two nuclear spin qubits.

These experiments were significant milestones towards implementation of HBAC. They demonstrated high control fidelity to realize HBAC to prepare an ancilla qubit whose polarization is higher than the cold bath polarization. The control tools are available, but what remains a challenge is to identify a system with a big enough number of qubits and a heat-bath with low polarization; or even find a better way to couple the qubits to the heat-bath to remove entropy.

Chapter 4

Achievable Polarization for Heat-Bath Algorithmic Cooling

To understand the usefulness of HBAC in experiments, we need to understand the physical limits of cooling qubits in detail through compression/extraction of entropy. This limit has an important impact not only for the experimental realization of algorithmic cooling, but it is also very important from a microscopic thermodynamics point of view. In this context, the two very interesting questions are what is the achievable cooling when the initial state is maximally mixed, and how many iterations of the HBAC-steps would be needed to obtain a certain cooling, i.e. a certain required value of polarization.

We investigated the achievable polarization by analyzing the limit when no more entropy can be extracted from the system. In this chapter, we give an analytic form of the maximum polarization achievable for the case when the initial state of the qubits is totally mixed. Also, we give the corresponding steady state of the whole system. It is however possible to reach higher polarization while starting with certain states other than a mixed state, thus our result provides an achievable polarization. We also give the number of steps needed to get a specific required polarization.

4.1 Cooling Limit

The cooling limit corresponds to the moment at which it is not possible to continue extracting entropy from the computational qubit system, i.e. *when the state of the qubit system is not changed by the compression and refresh steps*. The system achieves this limit asymptotically,

converging to a steady state where the following condition holds:

$$\rho = \rho'', \tag{4.1}$$

where ρ'' is the state of the qubit system after one HBAC iteration on ρ.

The state of the computational qubits, $\rho_{com} = \mathrm{Tr}_{m_{qubits}}(\rho)$, can be expressed as

$$diag(\rho_{com}) = (A_1, A_2, A_3, ..., A_{2d}), \tag{4.2}$$

where $diag(\rho)$ is the vector of the diagonal elements of ρ. From this and eq.(3.3), ρ'' will be described by

$$diag(\rho'') = (A_1, A_2, ..., A_{2d}) \otimes \frac{1}{2^m} (1 + \epsilon_b, 1 - \epsilon_b)^{\otimes m}. \tag{4.3}$$

In the cooling limit there is no operation that can compress any further the entropy of the computational qubits, or equivalently, the diagonal elements of ρ'' are already sorted in decreasing order. This will happen when we have the condition

$$A_i (1 - \epsilon_b)^m \geq A_{i+1} (1 + \epsilon_b)^m, \tag{4.4}$$

for $i = 1, 2, 3, ..., 2d - 1$, (see the next chapter for proof details). When this equation is satisfied, the entropy of the reset qubits will not increase anymore after compression and thus contact with the bath will not cool them. Thus, HBAC iterations will not modify the state anymore, leading to (4.1).

Note that this condition does not imply that there is a single steady state. In fact, it is possible to find different final states as a function of the initial state of the system. The most interesting steady state is given when the initial state is totally mixed, since it corresponds to the extreme case when the initial polarization is zero, and even better, because it is always possible to efficiently randomized a state experimentally. Therefore, that state can always be asymptotically reached.

4.2 Maximally mixed initial state

If we start with a maximally mixed state, it is possible to show that

$$A_i^t (1 - \epsilon_b)^m \leq A_{i+1}^t (1 + \epsilon_b)^m, \tag{4.5}$$

for $i = 1, 2, 3, ..., 2d - 1$, where t labels the number of HBAC iterations. This is true for the initial step, as $A_i = \frac{1}{2d}$ for all i at $t = 0$, but it turns out that it remains true for all subsequent iterations.

It is also possible to show that at each step the polarization of the target qubit never decreases, while the entropy of the reset qubits always increases beyond the one from the bath at each entropy compression step. Thus, the reset qubits always pump entropy out of the system into the bath, converging to a limit.

Comparing eq.(4.4) and eq.(4.5) indicates that the asymptotic state of the computational qubits can only go towards the equality

$$A_i^{\infty}\left(1-\epsilon_b\right)^m = A_{i+1}^{\infty}\left(1+\epsilon_b\right)^m, \tag{4.6}$$

for all $i = 1, 2, 3, ..., 2d-1$.

From (4.6) and the property $\mathrm{Tr}\left(\rho_{com}\right) = 1$, it is possible to find all the diagonal elements of ρ_{com}, which are as follows: $A_i^{\infty} = \frac{1-Q}{1-Q^{2d}}Q^{i-1}$, where $Q = \left(\frac{1-\epsilon_b}{1+\epsilon_b}\right)^m$. This result gives the exact solution of the steady state of the computational qubits, $\widetilde{\rho}_{com}$, for all values of the bath polarization:

$$diag\left(\widetilde{\rho}_{com}\right) = A_1^{\infty}\left(1, Q, Q^2, ..., Q^{2d-1}\right). \tag{4.7}$$

See the next chapter for details. (A special case of this result was presented in the paper [39], for $d = 2^{n'}$ and $m = 1$. However, their claim that this is the asymptotic limit for *all* HBAC methods is incorrect, as explained in chapter 6).

4.2.1 Asymptotic Polarization

From the steady state (eq. (4.7)), the asymptotic polarization of the target qubit is

$$\epsilon_{\mathbb{1}}^{\infty} = \frac{\left(1+\epsilon_b\right)^{md} - \left(1-\epsilon_b\right)^{md}}{\left(1+\epsilon_b\right)^{md} + \left(1-\epsilon_b\right)^{md}}. \tag{4.8}$$

The corresponding temperature of the target qubit will be $T_{steady} = \frac{1}{md}T_b\frac{\Delta E_t}{\Delta E_r}$ ($d = 2^{n'}$ when the scratch qudit is a string of n' qubits), here T_b is the temperature of the bath, and ΔE_t and ΔE_r are the energy gaps between the two energy levels of the target qubit, and the reset qubits, respectively. Our results agree with the third law of thermodynamics [40, 41].

For the case of using a string of qubits as the scratch qudit, the maximum achievable polarization of the j^{th} qubit will be $\epsilon_{max}^{(j)} = \frac{\left(1+\epsilon_b\right)^{m2^{j-1}} - \left(1-\epsilon_b\right)^{m2^{j-1}}}{\left(1+\epsilon_b\right)^{m2^{j-1}} + \left(1-\epsilon_b\right)^{m2^{j-1}}}$ (numbered from right to left, Fig. 3.1).

In the limit for low bath polarization, $\epsilon_b << 1/md$, the achievable asymptotic polarization is proportional to the dimension of the Hilbert space of the scratch qudit (or n' qubits), i.e. $\epsilon_{\mathbb{1}}^{\infty} \approx md\epsilon_b (= m2^{n'}\epsilon_b)$. As the value of ϵ_b increases beyond $1/md$, we observe a transition for

the asymptotic polarization. This is shown in Fig.4.1, as a function of the bath polarization for different number of qubits, using eq. (5.31). We can observe the transition noted by [20] and [5] at $\epsilon_b \sim 2^{-n}$, for $m = 1$, agreeing with simulations.

In order to see how $\epsilon_{\mathbb{1}}^{\infty}$ approaches 1, we use $\Delta_{max} = 1 - \epsilon_{\mathbb{1}}^{\infty}$, and eq (5.31). Then,

$$\Delta_{max} = \frac{2}{e^{md\ln\left(\frac{1+\epsilon_b}{1-\epsilon_b}\right)} + 1} = \frac{2}{e^{m2^{n'}\ln\left(\frac{1+\epsilon_b}{1-\epsilon_b}\right)} + 1}. \tag{4.9}$$

This expression shows that the asymptotic polarization goes to 1 doubly exponentially in the number of qubits n' (or exponential as a function of the size of the Hilbert space d). In Fig. 4.1, we show $\epsilon_{\mathbb{1}}^{\infty}$ as a function of ϵ_b for different values of d, with $m = 1$.

Example image

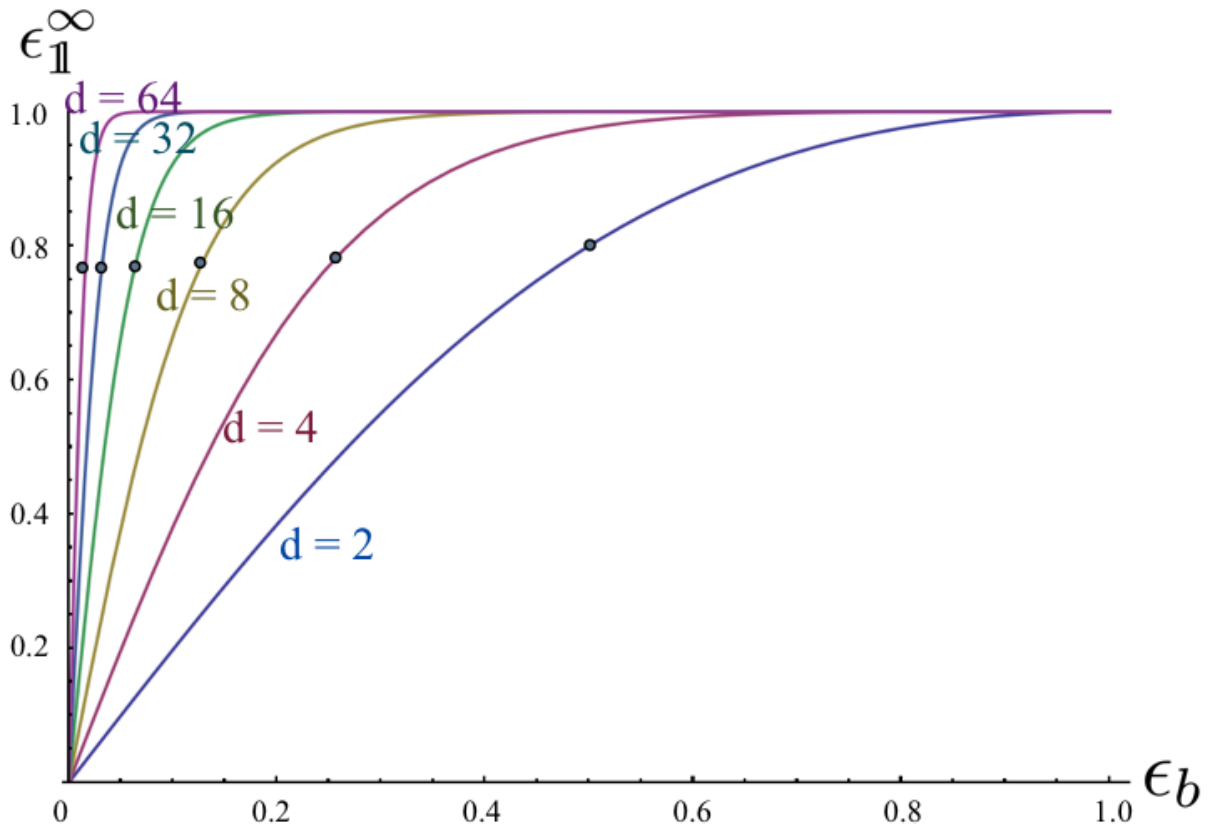

Figure 4.1: Asymptotic achievable polarization for the target qubit. This polarization increases double exponentially in the number of qubits as the scratch qudit, n'. The dots are located at the point of $\epsilon_{\mathbb{1}}^{\infty}$ which corresponds to the $\epsilon_b = \frac{1}{md}$, where the transition can be observed, for $d = 2$, 4, 8, 16, 32, and 64, and $m = 1$. (For ϵ_b smaller than that value, $\epsilon_{\mathbb{1}}^{\infty}$ is linear in ϵ_b.)

The asymptotic polarization $\epsilon_{\mathbb{1}}^{\infty}$ was obtained assuming the system qubits started in the completely mixed state. The same asymptotic polarization would be obtained if we start with a

different initial state that nevertheless obeys eq.(4.5). Numerical simulation indicates that this could also happens with some initial states not obeying eq.(4.5). But we can also find explicit examples of initial states that lead to asymptotic polarizations that are higher than eq.(5.31). As any state can be efficiently maximally randomized, it is always possible to reach the polarization given eq.(5.31) and maybe do better if the initial state is different.

4.2.2 Schulman's Physical-Limit Theorem

The steady state, eq. (4.7), is consistent with the limits of HBAC given by the theorem of Schulman et al. [6]. Their theorem provides an upper bound of the probability of having any basis state, concluding that no heat-bath method can increase that probability from its initial value, 2^{-n}, to more than $min\{2^{-n}e^{\epsilon 2^{n-1}}, 1\}$. Where ϵ is related to the polarization of the heat-bath as $\epsilon_b = \tanh\epsilon$, and n is the total number of qubits ($n = n' + 2$: $n' + 1$ computational qubits and one reset qubit).

We improved that theorem by finding the corresponding exact maximum probability, p_{max}. p_{max} is given by the probability of having the basis state $|00...0\rangle$ at the cooling limit: $p_{max} = A_1 \left(1 + \epsilon_b\right)/2$ (from eq. (4.7) and $\rho = \widetilde{\rho}_{com} \otimes \rho_{\epsilon_b}$). That expression can by written as a function of n and ϵ_b as follows $p_{max} = \frac{\epsilon_b}{1-\left(\frac{1-\epsilon_b}{1+\epsilon_b}\right)^{2^{n-1}}}$.

Fig. 4.2 shows both the upper bound proposed by Schulman (dashed lines) and the asymptotic value obtained here (thick lines), for different values of n. We can see that the bound is very close to the exact solution for small values of ϵ_b, but differ for large values of ϵ_b.

4.2.3 Number of steps needed to get $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$

We calculated the number of steps required to get a certain polarization for the three qubit case (m=1, d=2). For this, we studied the polarization evolution after each step of the PPA method on the system, starting from the total mixed state. The required quantum circuit to perform the PPA method is shown in Fig. 3.8.

Consider that the polarization of the first qubit is ϵ^t after the t^{th} iteration. Applying two more iterations, which corresponds to the 3qubit-round in Fig. 3.8, the polarization of the target qubit increases from ϵ^t to ϵ^{t+2} as follows:

$$\epsilon^{t+2} = 2ab\epsilon^t + \epsilon_b, \tag{4.10}$$

where $a = \frac{1+\epsilon_b}{2}$ and $b = \frac{1-\epsilon_b}{2}$.

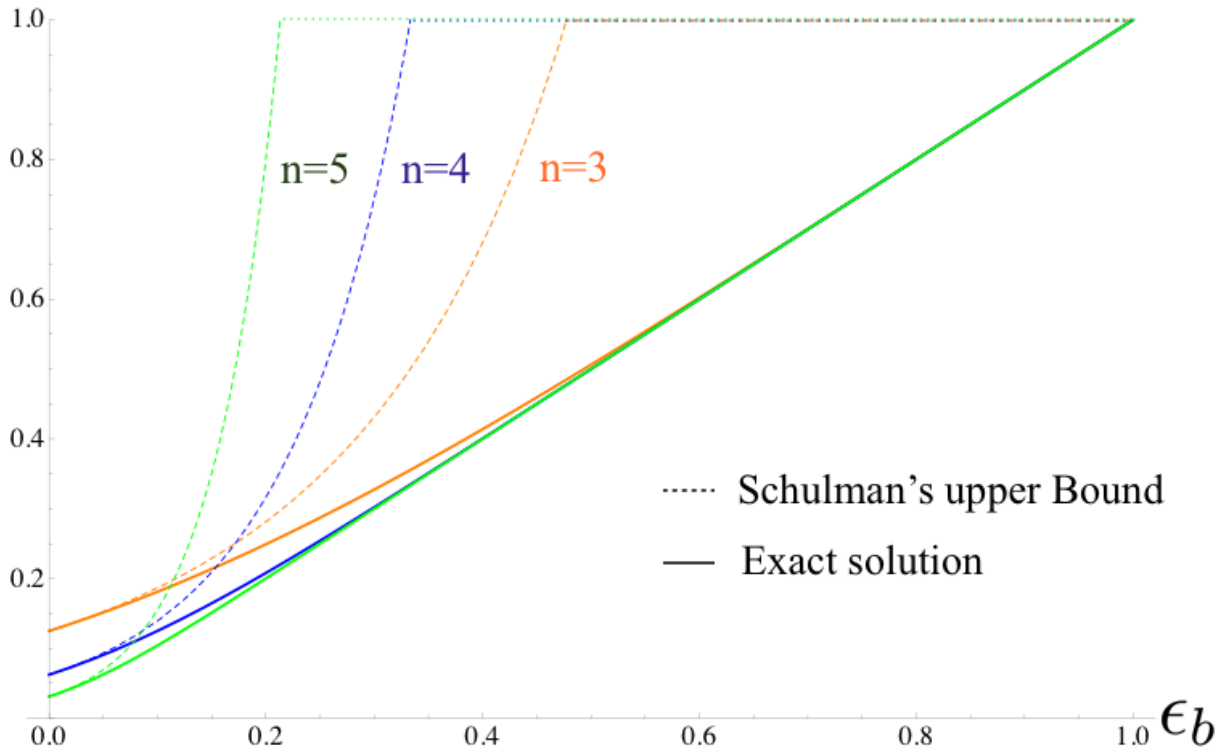

Figure 4.2: Upper limit of the probability of any basis state for the total n qubit system ($n = n' + 2$: $n' + 1$ computational qubits and one reset qubit). The dashed line corresponds to the Schulman's upper bound and the thick line to the exact asymptotic probability. Orange for $n = 3$, blue for $n = 4$, and Green for $n = 5$

Let t starts from 0, then $\epsilon^0 = \epsilon_b$ after the first iteration. From eq.(4.10), the polarization after applying j 3qubit-rounds can be written as

$$\epsilon^{t=2j} = \epsilon_{\mathbb{1}}^{\infty} - q^j \left(\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b\right), \tag{4.11}$$

where $q = \frac{1-\epsilon_b^2}{2}$. Using (5.31) with $d = 2$, we have that the corresponding asymptotic polarization $\epsilon_{\mathbb{1}}^{\infty} = \frac{2\epsilon_b}{1+\epsilon_b^2}$. From this equation we can find the number of steps needed to get to $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$,

$$N(\delta, \epsilon_b) = 2j = 2\frac{\log\left(\frac{\delta}{\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b}\right)}{\log q}. \tag{4.12}$$

The upper bound on the number of steps required to get polarization $\epsilon_{h,\delta} < \epsilon_{max}$ for the cases of a string of n qubits ($n' = n - 2$, $m = 1$) is

$$N_{upper-bound} = \prod_{k=1}^{k=[n'/2]} N(\delta_k, \epsilon_k), \tag{4.13}$$

where $\epsilon_{max} = \frac{(1+\epsilon_b)^{d/2}-(1-\epsilon_b)^{d/2}}{(1+\epsilon_b)^{d/2}+(1-\epsilon_b)^{d/2}}$; $\epsilon_k := f(\epsilon_{k-1}) - \delta_k$; $\epsilon_{h,\delta} = \epsilon_h$, with $h = [n'/2]$ (the integer part of $n'/2$); $f(\epsilon) = \frac{2\epsilon}{1+\epsilon^2}$; $N(\delta, \epsilon) = 2\frac{\log\left(\frac{\delta}{f(\epsilon_b)-\epsilon_b}\right)}{\log q}$; and $\epsilon_0 = \epsilon_b$. (See the next chapter for more details.)

Despite the simplicity and periodicity of the three qubits quantum circuit, it is complicated to generalize this for a bigger number of qubits. First, the entropy compression operation depends on the state of the system and, thus, is different in each iteration. Second, the number of gates needed in each iteration grows with the number of qubits.

Fig. 5.1 shows numerical simulations of the number of steps as a function of $\delta_{rel} = \frac{\epsilon_{\mathbb{1}}^{\infty}-\epsilon}{\epsilon_{\mathbb{1}}^{\infty}} = \delta/\epsilon_{\mathbb{1}}^{\infty}$. The simulations are consistent with the upper bound of the number of steps and with the

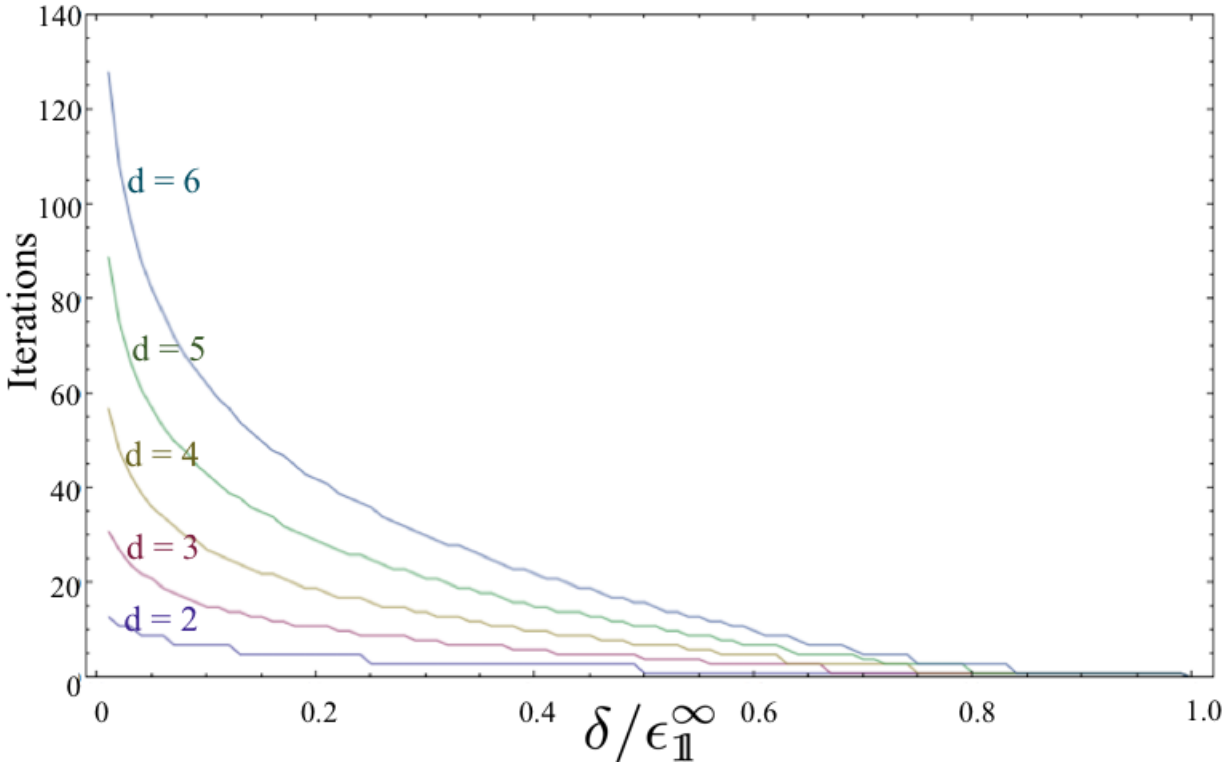

Figure 4.3: Number of PPA-iterations that are required to have polarization $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$ as a function of $\delta/\epsilon_{\mathbb{1}}^{\infty}$, for d=2, 3, 4, 5, and 6.

exact solution for the case of three qubits.

Chapter 5

Achievable Polarization Proofs

In this chapter, we explain in detail how to obtain the principal results of the previous chapter. First, we give the conditions of the cooling limit and the requirements to have a steady state. Then, we show that these conditions can be reached asymptotically when we start from the maximally mixed state. We derive the maximum polarization achievable when the initial state is totally mixed, and the corresponding temperature. Furthermore, we explain how to get the number of steps needed to have a certain polarization $\epsilon_{\mathbb{1}}^{\infty} - \delta$ (we give the exact solution for $n = 3$, and an upper bound for $n > 3$).

5.1 Cooling limit

In the cooling limit it is not possible to continue extracting entropy from the computational qubits. Thus, the corresponding state, ρ_{com}, will not change by applying the compression and refresh steps of HBAC.

The method to find this steady state is to consider the general form of ρ_{com}, and apply the two steps of the HBAC method to get ρ''_{com}. The conditions for the steady state are given by the equality of these states.

Assume that we start with a system in the totally mixed state. By applying compression and refresh operations, the state remains diagonal. Thus, the state of the whole qubit system, ρ, can

be completely described by its diagonal elements,

$$diag(\rho) = \begin{bmatrix} p_1 \\ p_2 \\ . \\ . \\ . \\ p_D \end{bmatrix}, \tag{5.1}$$

where $diag(\rho)$ is the vector of the diagonal elements of ρ, and D is the dimension of the Hilbert space of the whole string of qubits ($D = 2d2^m$).

Applying HBAC, the state evolves through the following two steps:

Entropy Compression Step: $\rho \xrightarrow{Compress} \rho' = U\rho U^\dagger$**.** In the PPA, U sorts the diagonal elements of ρ in decreasing order, giving a ρ' with diagonal elements

$$p'_1 \geq p'_2 \geq ... \geq p'_{D-1} \geq p'_D. \tag{5.2}$$

The state of the computational qubits, ρ'_{com}, is given by

$$diag(\rho'_{com}) = diag(\mathrm{Tr}_m(\rho')) := \begin{bmatrix} A_1 \\ A_2 \\ . \\ . \\ . \\ A_{2d} \end{bmatrix}, \tag{5.3}$$

where $\mathrm{Tr}_m()$ is the partial trace operation over the m reset qubits, and $A_k = \sum_{j=j_{k_0}}^{j_k} p'_j$, with $j_{k_0} = (k-1)2^m + 1$ and $j_k = k2^m$. This, with eq. (5.2), implies that

$$A_1 \geq A_2 \geq ... \geq A_{2d-1} \geq A_{2d}. \tag{5.4}$$

Refresh Step: $\rho' \xrightarrow{Refresh} \rho'' = \mathrm{Tr}_m(\rho') \otimes \rho_{\epsilon_b}^{\otimes m}$**,** where $\rho_{\epsilon_b} = \frac{1}{2}\begin{pmatrix} 1+\epsilon_b & 0 \\ 0 & 1-\epsilon_b \end{pmatrix}$ is the state of a qubit with heat-bath polarization ϵ_b.

After these compression and refresh steps, the state of the total qubit system, ρ'', will be

described by

$$diag\left(\rho''\right) = \begin{bmatrix} A_1 \\ A_2 \\ . \\ . \\ . \\ A_{2d-1} \\ A_{2d} \end{bmatrix} \otimes \frac{1}{2^m} \begin{pmatrix} 1+\epsilon_b \\ 1-\epsilon_b \end{pmatrix}^{\otimes m} . \tag{5.5}$$

In the cooling limit there is no operation that can compress any further the entropy of the computational qubits, or equivalently, the diagonal elements of ρ'' are already sorted in decreasing order.

Starting with the simplest case, m=1 (using only one reset qubit), the $diag(\rho'')$ is as follows (from eq.(5.5)):

$$diag\left(\rho''\right) = \frac{1}{2} \begin{bmatrix} A_1\left(1+\epsilon_b\right) \\ A_1\left(1-\epsilon_b\right) \\ A_2\left(1+\epsilon_b\right) \\ A_2\left(1-\epsilon_b\right) \\ . \\ . \\ . \\ A_{2d}\left(1+\epsilon_b\right) \\ A_{2d}\left(1-\epsilon_b\right) \end{bmatrix} . \tag{5.6}$$

If the elements of ρ'' are already sorted, it implies that

$$A_i(1-\epsilon_b) \geq A_{i+1}(1+\epsilon_b), \tag{5.7}$$

for all $i = 1, 2, ..., 2d-1$, which is a condition required for a steady state under the PPA-HBAC. Note that there are many solutions to this set of equations, and, not surprisingly, many steady states of HBAC.

Now, we will show that we can reach a steady state if we start from the totally mixed state.

Let A_i^t be the evolution of A_i after t iterations of the PPA-HBAC, with $A_i^0 = \frac{1}{2d}$ when the initial state is totally mixed. Interestingly, we have

$$A_i^0(1-\epsilon_b) \leq A_{i+1}^0(1+\epsilon_b), \tag{5.8}$$

for all $i = 1, 2, ..., 2d-1$. Note that it is a less than equal sign in distinction from (5.7). We will show that if (5.8) is true at $t = 0$, it will be true for all future steps t. Moreover, we will also

show that if (5.8) is obeyed, the rounds of HBAC keep cooling the computational qubits. Thus, the state of the system reaches asymptotically the condition of (5.7) with the equality.

We will prove that if we have $\frac{A_i^t}{A_{i+1}^t} \leq \frac{1+\epsilon_b}{1-\epsilon_b}$ for all $i = 1, 2, ..., 2d-1$ at a given moment t, then after an iteration of HBAC we will have $\frac{A_i^{t+1}}{A_{i+1}^{t+1}} \leq \frac{1+\epsilon_b}{1-\epsilon_b}$.

Let ρ_{com}^t be the state of the computational qubits after t iterations. Then, the density matrix of the total qubit system state will be given by $\rho^t = \rho_{com}^t \otimes \rho_{\epsilon_b}$, just after a refresh step. Thus, the total state is as follows:

$$diag(\rho^t) = \begin{bmatrix} p_1^t \\ p_2^t \\ p_3^t \\ p_4^t \\ p_5^t \\ p_6^t \\ . \\ . \\ . \\ p_{2(2d)-1}^t \\ p_{2(2d)}^t \end{bmatrix} = \frac{1}{2} \begin{bmatrix} A_1^t\,(1+\epsilon_b) \\ A_1^t\,(1-\epsilon_b) \\ A_2^t\,(1+\epsilon_b) \\ A_2^t\,(1-\epsilon_b) \\ A_3^t\,(1+\epsilon_b) \\ A_3^t\,(1-\epsilon_b) \\ . \\ . \\ . \\ A_{2d}^t\,(1+\epsilon_b) \\ A_{2d}^t\,(1-\epsilon_b) \end{bmatrix}. \tag{5.9}$$

The elements of ρ^t can be written as

$$p_{2i-1}^t = A_i^t(1+\epsilon_b)/2, \text{and} \tag{5.10}$$

$$p_{2i}^t = A_i^t(1-\epsilon_b)/2, \tag{5.11}$$

for $i = 1, 2, ..., 2d$.

For the next step, we have to compress ρ^t to get ρ^{t+1}, i.e. we have to sort the diagonal elements of ρ^t in decreasing order.

Observe that the elements with factor $(1+\epsilon_b)$ (the blue elements in (5.9)) are already in descending order, since $A_1^t \geq A_2^t \geq ... \geq A_{2d}^t$. Therefore, during the compression step, these elements can be moved to different entries of the diagonal matrix from the initial ones, but they will have the same order among them (because they are already sorted). It is similar for the elements with factor $(1-\epsilon_b)$ (the red elements).

Assuming $\frac{A_i^t}{A_{i+1}^t} \leq \frac{1+\epsilon_b}{1-\epsilon_b}$, as we have in the initial state, implies that the blue elements are going to go up at least one row, except for $A_1^t(1+\epsilon_b)$ which stays in the same position. Similarly,

the red elements are going to go down at least one row, except for $A^t_{2d}(1-\epsilon_b)$ which stays in the same position.

Considering this element movement, we can conclude that the elements of ρ^{t+1} will satisfy the following inequalities:

$$A^t_{i-1}(1-\epsilon_b)/2 \leq p^{(t+1)}_{2i-1} \leq A^t_i(1+\epsilon_b)/2, \text{and} \tag{5.12}$$

$$A^t_i(1-\epsilon_b)/2 \leq p^{(t+1)}_{2i} \leq A^t_{i+1}(1+\epsilon_b)/2, \tag{5.13}$$

for $i = 2, 3, ..., 2d-1$.

The new computational state, $\rho^{t+1}_{com} = \mathrm{Tr}_m(\rho^{t+1})$, will have diagonal elements $A^{t+1}_i = p^{(t+1)}_{2i-1} + p^{(t+1)}_{2i}$. From this and (5.12)-(5.13), we have

$$(A^t_{i-1} + A^t_i)(1-\epsilon_b)/2 \leq A^{(t+1)}_i \leq (A^t_i + A^t_{i+1})(1+\epsilon_b)/2, \tag{5.14}$$

for $i = 2, 3, ..., 2d-1$. For the first and last diagonal elements of ρ_{com} ($i = 1$ and $i = 2d$), we know exactly their corresponding values,

$$A^{t+1}_1 = (A^t_1 + A^t_2)(1+\epsilon_b)/2, \text{and} \tag{5.15}$$

$$A^{t+1}_{2d} = (A^t_{2d-1} + A^t_{2d})(1-\epsilon_b)/2. \tag{5.16}$$

These last three equations imply that $\frac{A^{t+1}_i}{A^{t+1}_{i+1}}$ satisfy the following inequality:

$$\frac{A^{t+1}_i}{A^{t+1}_{i+1}} \leq \frac{A^t_i(1+\epsilon_b) + A^t_{i+1}(1+\epsilon_b)}{A^t_i(1-\epsilon_b) + A^t_{i+1}(1-\epsilon_b)} = \frac{1+\epsilon_b}{1-\epsilon_b}, \tag{5.17}$$

for all $i = 1, 2, ..., 2d-1$, as we claimed.

5.1.1 Increasing purity

We now show that starting in the totally mixed state and applying steps of HBAC, the system will asymptotically go to a state that satisfies the equality in (5.7). To show this, we will prove that the target qubit (the spin$-1/2$) is cooled after each iteration of HBAC, and the reset qubit keeps extracting entropy from the system (cooling the system) after each iteration. All this drives asymptotically the initial state to the steady state.

Consider the state of the system after t iterations, (state of the eq. (5.9)). Then, the reduced density matrix for the target qubit is

$$diag(\rho^t_{target}) = \begin{bmatrix} \rho^t_{00_{target}} \\ \rho^t_{11_{target}} \end{bmatrix}, \tag{5.18}$$

where $\rho^t_{00_{target}} = \sum_{i=1}^{2d} p_i^t = \sum_{i=1}^{d} A_i^t$, and $\rho^t_{11_{target}} = 1 - \rho^t_{00_{target}}$.

Since the compression step reorders the diagonal elements of ρ^t in decreasing order, it is clear that the first $2d$ elements of the new state, ρ^{t+1}, will satisfy $\sum_{i=1}^{2d} p_i^{t+1} \geq \sum_{i=1}^{2d} p_i^t$,

$$\implies \rho^{t+1}_{00_{target}} \geq \rho^t_{00_{target}}. \tag{5.19}$$

Therefore, the target qubit is always colder (or remains same) after each iteration of HBAC.

On the other hand, the reset qubit, which has reduced density matrix ρ_r^t when the total system has state ρ^t, will be

$$diag(\rho_r^{t+1}) = \begin{bmatrix} \rho^{t+1}_{00_r} \\ \rho^{t+1}_{11_r} \end{bmatrix}, \tag{5.20}$$

where $\rho^{t+1}_{00_r} = \sum_{i=1}^{2d} p^{t+1}_{2i-1}$. This equation, with (5.12) and (5.10), gives

$$\rho^{t+1}_{00_r} = \sum_{i=1}^{2d} p^{t+1}_{2i-1} \leq \sum_{i=1}^{2d} A_i^t(1+\epsilon_b)/2 = (1+\epsilon_b)/2. \tag{5.21}$$

Therefore, the reset qubit will always be hotter than the bath after the compression step of HBAC as long as we do not reach the equality. This implies that the reset qubit always extracts entropy from the total system when it is brought into contact with the heat-bath. The system is cooled in every iteration of the refresh step, with a smaller and smaller amount of entropy extracted, going asymptotically the cooling limit.

The two elements above show that, starting from the totally mixed state, we will converge to the equality of (5.7). At this limit, the steady state of the computational qubits should have elements which satisfy

$$\frac{A^\infty_{i+1}}{A^\infty_i} = \frac{1-\epsilon_b}{1+\epsilon_b} \equiv Q. \tag{5.22}$$

Using (5.22) and $Tr(\rho_{com}) = 1$, it is possible to find the exact solution of each A_i^∞:

$$A_i^\infty = \frac{1-Q}{1-Q^{2d}} Q^{i-1}, \tag{5.23}$$

and therefore the analytical solution of the steady state of the computational qubits will be

$$diag\left(\rho_{com}^{\infty}\right) = A_1^{\infty} \begin{bmatrix} 1 \\ Q \\ Q^2 \\ . \\ . \\ . \\ Q^{2d-1} \end{bmatrix}. \tag{5.24}$$

5.1.2 Asymptotic Polarization of the target qubit for one and multiple reset qubits

Using eq.(5.24), the reduced density matrix of the target qubit in the cooling limit is given by

$$diag(\rho_{target}^{\infty}) = A_1^{\infty} \sum_{i=0}^{d-1} Q^i \begin{bmatrix} 1 \\ Q^d \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+\epsilon_{\mathbb{1}}^{\infty} \\ 1-\epsilon_{\mathbb{1}}^{\infty} \end{bmatrix}, \tag{5.25}$$

where $\epsilon_{\mathbb{1}}^{\infty}$ is the asymptotic polarization of the target qubit when we start with the maximally mixed state.

From this equation we can derive:

$$\epsilon_{\mathbb{1}}^{\infty} = \frac{(1+\epsilon_b)^d - (1-\epsilon_b)^d}{(1+\epsilon_b)^d + (1-\epsilon_b)^d}, \tag{5.26}$$

where d is the dimension of the Hilbert space of the scratch qudit ($d = 2l+1$ if we use a spin$-l$, or $d = 2^{n'}$ if we use a string of n' qubits).

Now, if we generalize to the case $m > 1$, we have that the state of the m reset qubits is given by

$$diag(\rho_{\epsilon_b}^{\otimes m}) = \begin{pmatrix} 1+\epsilon \\ 1-\epsilon \end{pmatrix}^{\otimes m} = \begin{pmatrix} (1+\epsilon)^m \\ . \\ . \\ . \\ (1-\epsilon)^m \end{pmatrix}, \tag{5.27}$$

where $(1+\epsilon_b)^m$ is the biggest element, and $(1-\epsilon_b)^m$ the smallest one, which correspond to the first entry and the last entry, respectively. Observe that in general the diagonal elements of $\rho_{\epsilon_b}^{\otimes m}$ are not in decreasing order.

From eq. (5.5), ρ'' is as follows:

$$diag(\rho'') = \begin{pmatrix} \boxed{\begin{matrix} A_1\,(1+\epsilon_b)^m \\ \vdots \\ A_1\,(1-\epsilon_b)^m \end{matrix}} \\ \boxed{\begin{matrix} A_2\,(1+\epsilon_b)^m \\ \vdots \\ A_2\,(1-\epsilon_b)^m \end{matrix}} \\ \vdots \\ \boxed{\begin{matrix} A_i\,(1+\epsilon_b)^m \\ \vdots \\ A_i\,(1-\epsilon_b)^m \end{matrix}} \\ \boxed{\begin{matrix} A_{i+1}\,(1+\epsilon_b)^m \\ \vdots \\ A_{i+1}\,(1-\epsilon_b)^m \end{matrix}} \\ \vdots \\ \boxed{\begin{matrix} A_{2d}\,(1+\epsilon_b)^m \\ \vdots \\ A_{2d}\,(1-\epsilon_b)^m \end{matrix}} \end{pmatrix}$$

First, notice that any swap between two elements within the same box (which has the same factor A_i) will not improve the entropy compression on the computational qubits state. The reason is once the reset qubits are traced out, the permutation inside the same box contributes to the sum of the probabilities corresponding to same basis state of the computational qubits that they contributed before the compression.

Then, we are just interested in permuting elements to a different box from where they were previously, in particular the biggest element or smallest element of each box (to have the maximum entropy compression). At the cooling limit, there is no operation that can improve the compression, or equivalently, the elements (just taking the largest and smallest of each box) are already sorted.

Following the same reasoning to the case when $m = 1$, the steady state should have elements which hold:

$$A_i^{\infty}(1-\epsilon_b)^m \geq A_{i+1}^{\infty}(1+\epsilon_b)^m. \tag{5.28}$$

Moreover, similarly to the case of $m = 1$, the inequality $\frac{A_i}{A_{i+1}} \leq \frac{(1+\epsilon_b)^m}{(1-\epsilon_b)^m}$ cannot be inverted by applying the steps of HBAC. Therefore, if we start with a totally mixed state (which holds the last inequality mentioned), the steady state should have elements which hold

$$A_i^{\infty}(1-\epsilon_b)^m = A_{i+1}^{\infty}(1+\epsilon_b)^m. \tag{5.29}$$

Then, the analytical solution of the steady state of the computational qubits will be

$$diag\left(\rho_{com}^{\infty}\right) = A_1^{\infty} \begin{bmatrix} 1 \\ Q^m \\ Q^{2m} \\ . \\ . \\ . \\ Q^{(2d-1)m} \end{bmatrix}. \tag{5.30}$$

Similarly, the maximum achievable polarization using m reset qubits will be

$$\epsilon_{\mathbb{1}}^{\infty} = \frac{(1+\epsilon_b)^{md} - (1-\epsilon_b)^{md}}{(1+\epsilon_b)^{md} + (1-\epsilon_b)^{md}}. \tag{5.31}$$

Note that a similar polarization would be obtained if we start with a different initial state but which obeys eq.(5.8). Numerical simulation indicate that this could also happens with some initial states not obeying eq.(5.8). Finally, we can give explicit examples of initial states that lead to an asymptotic polarization higher than eq.(5.31).

5.1.3 Temperature in the cooling limit

The state of the heat-bath in thermal equilibrium, temperature T_b, is given by

$\rho_b = \frac{1}{e^{\Delta E_b/2kT_b} + e^{-\Delta E_b/2kT_b}} \begin{pmatrix} e^{\Delta E_b/2kT_b} & 0 \\ 0 & e^{-\Delta E_b/2kT_b} \end{pmatrix}$, where ΔE_b is the energy gap between the two energy levels of a qubit from the bath.

Then, the heat-bath polarization corresponds to $\epsilon_b = \tanh\left(\frac{\Delta E_b}{2kT_b}\right)$, or equivalently,

$$\frac{\Delta E_b}{2kT_b} = \frac{1}{2}\log\left[\frac{1+\epsilon_b}{1-\epsilon_b}\right]. \tag{5.32}$$

Similarly for the target qubit in the steady state at temperature T_{steady}, we will have $\frac{\Delta E_t}{2kT_{steady}} = \frac{1}{2}\log\left[\frac{1+\epsilon_{\mathbb{1}}^{\infty}}{1-\epsilon_{\mathbb{1}}^{\infty}}\right]$, where ΔE_t is the energy gap of the two energy levels of the target qubit. From this and eq.(5.31), we can obtain the temperature in the cooling limit,

$$T_{steady} = \left(\frac{1}{md}\right) T_b \left(\frac{\Delta E_t}{\Delta E_b}\right), \tag{5.33}$$

$d = 2^{n'}$ when the scratch qudit is a string of n' qubits ($n'+1$ computational qubits).

The PPA-HBAC method is in line with the third law of thermodynamics, which says that "it is impossible by any procedure, no matter how idealized, to reduce any assembly to absolute zero temperature in a finite number of operations" [40, 41]. Indeed, the evolution of the state of the system goes asymptotically to a steady state, which has non zero temperature for a finite number of qubits. The limit when the temperature is exactly zero corresponds to the case of having an infinite number of qubits. Since the number of gates needed grows with the number of qubits, the operations required to achieve temperature zero will be infinite.

Although the algorithm keeps cooling the target qubit at each time, it does so with a smaller and smaller amount of entropy extracted, asymptotically reaching the steady state of non-zero temperature. This is in agreement with the third law of thermodynamics.

5.1.4 Polarization of different computational qubits

Consider the case of having a string of n' qubits as scratch qubit. Let's label the qubits from right to left, as it is shown in Fig. 1 in the paper.

We can obtain the polarization of each qubit from the steady state (5.24). We already showed how to get the polarization of the target qubit. If we trace out the target qubit from the computational qubits, we can repeat the same calculations to get the polarization of the neighbor qubit in the string (which is labeled as qubit n') since this qubit will be now the first from the left.

The state of the computational qubits without the target qubit is

$$diag(\rho_{target}^{\infty}) = \mathrm{Tr}_{target}(\rho_{com}^{\infty}) = \begin{bmatrix} A_1^{\infty} + A_{d+1}^{\infty} \\ A_2^{\infty} + A_{d+2}^{\infty} \\ \cdot \\ \cdot \\ \cdot \\ A_d^{\infty} + A_{2d}^{\infty} \end{bmatrix}. \tag{5.34}$$

Let B_i be the ith element of the $diag(\rho^{\infty}_{target})$, i.e. $B_i = A^{\infty}_i + A^{\infty}_{d+i}$. From eq. (5.23), $B_i = A^{\infty}_1 Q^{i-1} + A^{\infty}_1 Q^{d+i-1} = A^{\infty}_1 (1+Q^d) Q^{i-1}$. Thus, $B_i = kQ^{i-1}$, where $k = A^{\infty}_1(1+Q^d)$. Comparing B_i with eq(5.23), we see that this state has the same form of the state eq. (5.24), but with Hilbert space dimension $d/2$. Thus, the asymptotic polarization of the $n'th$ qubit is

$$\epsilon^{(n')}_{max} = \frac{(1+\epsilon_b)^{md/2} - (1-\epsilon_b)^{md/2}}{(1+\epsilon_b)^{md/2} + (1-\epsilon_b)^{md/2}} \tag{5.35}$$

where $d = 2^{n'}$.

Similarly, we can get the polarization of the $(n'-1)^{th}$ qubit, and so on. Then, the polarization of the j^{th} qubit will be

$$\epsilon^{(j)}_{max} = \frac{(1+\epsilon_b)^{m2^{j-1}} - (1-\epsilon_b)^{m2^{j-1}}}{(1+\epsilon_b)^{m2^{j-1}} + (1-\epsilon_b)^{m2^{j-1}}}. \tag{5.36}$$

5.2 Number of steps needed to get $\epsilon = \epsilon^{\infty}_{\mathbb{1}} - \delta$

5.2.1 Analytical result for a string of three qubits (m=1, d=2).

The quantum circuit required to perform the PPA-HBAC on three qubits initially in the total mixed state is showed in Fig.3.8. This circuit shows the operations required for the first five iterations (each iteration consists of a refresh step and an entropy compression step). Subsequent iterations gates are the alternate repetition of the second and third iterations gates in Fig.3.8. The application of those two iterations will be referred as a 3qubit-round.

In order to know the effect of one 3qubit-round on the system, consider the state of the computational qubits at a given moment,

$$diag(\rho^t_{com}) = \begin{bmatrix} A^t_1 \\ A^t_2 \\ A^t_3 \\ A^t_4 \end{bmatrix}, \tag{5.37}$$

and the total system as $\rho^t = \rho^t_{com} \otimes \rho_{\epsilon_b}$. The polarization of the target qubit, ϵ^t, can be obtained from its reduced density matrix, $diag(\rho^t_{target}) = \begin{bmatrix} A^t_1 + A^t_2 \\ A^t_3 + A^t_4 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1+\epsilon^t \\ 1-\epsilon^t \end{bmatrix}$

$$\implies \epsilon^t = 2(A^t_1 + A^t_2) - 1. \tag{5.38}$$

In the first iteration of the 3qubit-round, the compression gate swaps the scratch qubit and the reset qubit. This swap can be performed by applying the unitary matrix shown in Fig.3.1.1, thus

$$diag(\rho^t) = \frac{1}{2}\begin{bmatrix} A_1^t\,(1+\epsilon_b) \\ A_1^t\,(1-\epsilon_b) \\ A_2^t\,(1+\epsilon_b) \\ A_2^t\,(1-\epsilon_b) \\ A_3^t\,(1+\epsilon_b) \\ A_3^t\,(1-\epsilon_b) \\ A_4^t\,(1+\epsilon_b) \\ A_4^t\,(1-\epsilon_b) \end{bmatrix} \Longrightarrow \frac{1}{2}\begin{bmatrix} A_1^t\,(1+\epsilon_b) \\ A_2^t\,(1+\epsilon_b) \\ A_1^t\,(1-\epsilon_b) \\ A_2^t\,(1-\epsilon_b) \\ A_3^t\,(1+\epsilon_b) \\ A_4^t\,(1+\epsilon_b) \\ A_3^t\,(1-\epsilon_b) \\ A_4^t\,(1-\epsilon_b) \end{bmatrix}. \tag{5.39}$$

Then, the density matrix of the computational qubits after the first iteration of the 3qubit-round is

$$diag(\rho_{com}^{t+1}) = \frac{1}{2}\begin{bmatrix} (A_1^t + A_2^t)\,(1+\epsilon_b) \\ (A_1^t + A_2^t)\,(1-\epsilon_b) \\ (A_3^t + A_4^t)\,(1+\epsilon_b) \\ (A_3^t + A_4^t)\,(1-\epsilon_b) \end{bmatrix}. \tag{5.40}$$

In the second iteration of the 3qubit-round, the compression step is performed by applying the unitary matrix shown in Fig.3.6. In this step we obtain ρ^{t+2},

$$diag(\rho^{t+2}) = \frac{1}{4}\begin{bmatrix} (A_1^t + A_2^t)\,(1+\epsilon_b)^2 \\ (A_1^t + A_2^t)\,(1+\epsilon_b)\,(1-\epsilon_b) \\ (A_1^t + A_2^t)\,(1-\epsilon_b)\,(1+\epsilon_b) \\ (A_3^t + A_4^t)\,(1+\epsilon_b)^2 \\ (A_1^t + A_2^t)\,(1-\epsilon_b)^2 \\ (A_3^t + A_4^t)\,(1+\epsilon_b)\,(1-\epsilon_b) \\ (A_3^t + A_4^t)\,(1-\epsilon_b)\,(1+\epsilon_b) \\ (A_3^t + A_4^t)\,(1-\epsilon_b)^2 \end{bmatrix}. \tag{5.41}$$

From this state, with the normalization property of the density matrix and (5.38), we can obtain the new polarization of the target qubit,

$$\epsilon^{t+2} = 2ab\epsilon^t + \epsilon_b, \tag{5.42}$$

where $a = \frac{1+\epsilon_b}{2}$ and $b = \frac{1-\epsilon_b}{2}$.

Let $t = 0$ (just after the iteration 0 which swaps the target qubit and the reset qubit, Fig.3.8), then the polarization of the target qubit at that moment will be $\epsilon^0 = \epsilon_b$. From eq.(5.42), we can get the exact polarization after each 3qubit-round, i.e. every two iterations,

$$\epsilon^{t=2j} = \frac{2\epsilon_b}{1+\epsilon_b^2} - q^j \left(\frac{2\epsilon_b}{1+\epsilon_b^2} - \epsilon_0 \right), \tag{5.43}$$

where $q = \frac{1-\epsilon_b^2}{2}$. From (5.31), the asymptotic polarization for this case is $\epsilon_{\mathbb{1}}^{\infty} = \frac{2\epsilon_b}{1+\epsilon_b^2}$, thus eq.(5.43) can be written as

$$\epsilon^{t=2j} = \epsilon_{\mathbb{1}}^{\infty} - q^j \left(\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b \right). \tag{5.44}$$

Since $q < 1$, $\epsilon^t \to \epsilon_{\mathbb{1}}^{\infty}$ when we increase j.

We can use (5.44) to know the number of rounds t needed to achieve polarization $\epsilon_{\mathbb{1}}^{\infty} - \delta$. From Eq. (5.44), we have $\delta = q^j \left(\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b \right)$, then the number of rounds required will be

$$N(\delta, \epsilon_b) := t = 2 \frac{\log\left(\frac{\delta}{\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b} \right)}{\log q}, \tag{5.45}$$

to get polarization

$$\epsilon_\delta(\epsilon_b, \delta) := \epsilon_{\mathbb{1}}^{\infty} - \delta = \frac{2\epsilon_b}{1+\epsilon_b^2} - \delta. \tag{5.46}$$

5.2.2 Numerical results

Let $\delta_{rel} = \frac{\epsilon_{\mathbb{1}}^{\infty} - \epsilon}{\epsilon_{\mathbb{1}}^{\infty}} = \delta / \epsilon_{\mathbb{1}}^{\infty}$. Fig.5.1 shows simulations of the number of refresh steps needed to achieve a polarization $\epsilon = \epsilon_{\mathbb{1}}^{\infty} (1 - \delta_{rel})$ as function of δ_{rel} for different values of d. The exact solution of number of steps needed for the 3 qubit case is consistent with the results from the simulations.

Figure 5.1: Number of iterations needed to achieve polarization $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$ as a function of $\delta / \epsilon_{\mathbb{1}}^{\infty}$, for d=2, 3, 4, 5, and 6.

5.2.3 Upper bound of the number of steps to get a certain polarization, for n qubits

Consider a string of $n' + 1$ computational qubits, numbered as in Fig. 1 in the paper, and one reset qubit, all starting in totally mixed state. Applying the compression for three qubits, using the reset qubit and qubit 1 to cool qubit 2, we can increase the polarization of qubit 2 to $\epsilon_1 = \epsilon_\delta(\epsilon_b, \delta)$ in $N_1 = N(\delta, \epsilon_b)$ steps, from (5.45) and (5.46).

After this preparation of qubit 2, we can swap it with qubit 3, and then prepare again qubit 2. We can apply again the compression for three qubits, but now using qubits 2 and 3 to cool qubit 4. In this case, we will need $N_2 = N(\delta, \epsilon_1) \cdot N_1$ number of steps to get polarization $\epsilon_2 = \epsilon_\delta(\epsilon_1, \delta)$ on qubit 4.

We can iterate this idea to use qubit 4 and qubit 5 to cool qubit 6, getting that we need $N_3 = N(\delta, \epsilon_2) \cdot N_2$ number of steps to achieve polarization $\epsilon_3 = \epsilon_\delta(\epsilon_2, \delta)$, and so on.

Since this is not the optimal compression (in terms of entropy extraction, under the assumption that the refresh step re-thermalizes the reset qubits to the heat-bath temperature), this number of iterations gives an upper bound of the optimal number given by PPA. The upper bound is $N_{upper-bound} = \prod_{k=1}^{k=[n'/2]} N(\delta, \epsilon_k)$, to achieve polarization $\epsilon < \epsilon_{max}$ on the target qubit, where $\epsilon_{max} = \epsilon_{\mathbb{1}}^{\infty} = \frac{(1+\epsilon_b)^{d/2} - (1-\epsilon_b)^{d/2}}{(1+\epsilon_b)^{d/2} + (1-\epsilon_b)^{d/2}}$, and $\epsilon = \epsilon_\delta(\epsilon_{h-1}, \delta)$ with $\epsilon_0 = \epsilon_b$, and $h = [n'/2]$ (the integer part of $n'/2$).

Chapter 6

State-reset as refresh step

There are different ways to couple the quantum system with a heat-bath to remove entropy, which can be used in the refresh step of HBAC. In particular, in the PPA method, the refresh step re-thermalizes the reset qubits to the heat-bath temperature, which is equivalent to swap these qubits with qubits from the bath. Under this kind of refreshing procedure, it has been proved that the PPA gives the optimal physical cooling in terms of entropy extraction [5, 6]. However, we found that there could be other kind of couplings that might give a better polarization than the one obtained by the PPA. In this chapter, we presented an example of one type of coupling which can surpass the PPA for the two qubit case. The content of this chapter was presented as a comment on the paper [39], where the authors claimed to have established "the fundamental limit of cooling for *all* HBAC techniques" (italics are ours). We show that this claim is incorrect by giving a counterexample.

For two qubits (one target qubit, which is going to be cooled, and one reset qubit), starting in the totally mixed state, the PPA gives a steady state with the qubits at the temperature of the bath and no polarization gain (above the one from the bath) is observed. The first refresh step polarizes the reset qubit, then the first PPA entropy compression transfers that polarization to the target qubit. The reset qubit is then in a fully mixed state and can be re-polarized by a thermal contact with the heat-bath. It turns out that after these steps, the diagonal terms are already ordered with non-increasing probability (SORT), such that the PPA does not increase the polarization anymore. We thus end up with two qubits in a thermal state, the same as the bath.

In a recent paper[42], Jun Li and collaborators studied the efficiency of Liouville space polarization transfer in the presence of a bath and showed cases/experiments where utilizing relaxation effects does offer an enhancement. In looking at the maximum polarization (or purity), they (re)-discovered that it is possible to enhance the polarization of one of two qubits beyond the bath polarization in presence of relaxation and cross relaxation of the quantum system.

6.1 Nuclear Overhauser Effect

It is possible to enhance the polarization of one spin (qubit) at the expense of a second spin (qubit) when their coupling to the bath leads to cross relaxation. This effect was discovered by Overhauser in 1953 [43] and has been observed many times experimentally.

6.1.1 NOE for two qubits

In the limit of low polarization, the expectation of the Z Pauli operator S_Z^1 ($\langle S_z^1 \rangle$), obeys the equation (see [44]):

$$\frac{d\langle S_z^1 \rangle}{dt} = -\rho_1(\langle S_z^1 \rangle - \langle S_z^1 \rangle_0) - \sigma(\langle S_z^2 \rangle - \langle S_z^2 \rangle_0), \tag{6.1}$$

where $\langle S_z^i \rangle_0$ is the expectation of S_z^i at equilibrium when the other spin is not driven (not rotated), ρ_1 is the relaxation parameter for the first spin, and σ is the cross relaxation parameter.

It is possible to drive (rotate) the second spin so that on the relevant timescale (related to ρ_2 and σ) the expectation of $\langle S_z^2 \rangle \approx 0$. Then the steady state of eq.(6.1) implies that

$$\langle S_z^1 \rangle = \langle S_z^1 \rangle_0 + \frac{\sigma}{\rho_1} \langle S_z^2 \rangle_0. \tag{6.2}$$

Note that $\langle S_z^1 \rangle$ corresponds to the polarization of the first qubit, this gives an enhancement compared to what the PPA gives, as long as σ/ρ_1 is positive (which happens in nature). One way to understand the process from an algorithmic point of view is to realize that the cross relaxation effectively provides a state relaxation/equilibration ("state reset") between $|11\rangle$ and $|00\rangle$, without touching the other states, analogous to the qubit reset. This form of reset accompanied by a rotation of the second qubit can however boost the polarization of the first qubit beyond what would be obtained by a qubit reset from the bath as in the PPA.

Thus the PPA, at least for two qubits, gives only a lower bound on maximum polarization achievable for HBAC. It is possible to generalize this idea to enhance the polarization of three qubits beyond the PPA, and the details will be provided in a forthcoming paper.

We have presented a Heat-Bath Algorithmic Cooling technique that can have a better polarization enhancement than the one obtained by the PPA. As mentioned our paper [1], the polarization achieved using the PPA should instead be interpreted as a lower bound on the maximum amount of polarization that can be achieved. Its importance is due to the simplicity of the PPA when the initial state is totally mixed or in an equilibrium thermal state. In this case, it is possible to get analytical results that describes both the steady state and its polarization from which we

can determine a variety of properties, e.g. to know how far it is from polarization of one and explicitly show how much resources are needed. It will be interesting to see if we can generalise the Overhauser effect and to know what advantages it can give as we increase the number of qubits.

Chapter 7

Conclusion

HBAC is a process to purify a number of qubits by removing entropy from them through entropy compression and cooling, using extra qubits and contact with a bath. We analyzed the cooling limits of HBAC using the PPA method, which gives the optimal physical cooling in terms of entropy extraction, under the assumption that the refresh step re-thermalizes the reset qubits with the heat-bath [5, 6].

We presented the physical conditions for the cooling limit, and from this, we derived the analytic steady state corresponding to a string of qubits at the cooling limit for the case when the initial state is totally mixed. The string of qubits consists of one qubit with a number of ancilla qubits (or a spin-l) and m reset qubits that can be put into contact with a bath with polarization ϵ_b.

We obtained the analytic expression for the maximum polarization achievable starting with a maximally mixed state, and its corresponding temperature. Furthermore, this amount of polarization can be achieved for other different initial states, as long as they obey the initial conditions given by eq.(4.5). This result is of fundamental importance not only from the quantum thermodynamics point of view, but it also provides valuable information for experimental applications. Since it is always possible to efficiently randomized a state, we can think of this asymptotic polarization as a general achievable bound of polarization.

Our exact expression for the achievable polarization improves the Schulman's theorem of the physical limits [5, 6], in which only an polarization upper bound was provided. From our analysis we can also understand the transition of behavior of the asymptotic polarization at $1/md$, observed by Moussa [20] and Schulman et al. [5]. Below this value, $\epsilon_{\mathbb{1}}^{\infty} \sim md\epsilon_b$, and above it will reach order unity double exponentially with the number of scratch qubits.

Moreover, we obtained the number of steps required to reach a specific required polarization.

We got the exact number for the three-qubit case and an upper bound for a general number of qubits n. This numbers are important in order to understand the usefulness of HBAC in experimental implementations.

Finally, we presented another way to refresh the system with different form of interaction with the bath using the NOE effect. This method can improve the polarization obtained by the PPA. We are currently investigating its corresponding maximum polarization. [1]

[1] This thesis is based on a paper accepted at Physical Review Letters on May 14 2015; it was also presented at the Institute for Quantum Computing on March 27 2014, and at the he 14th Annual Canadian Summer School on Quantum Information held at the University of Guelph (June 16-20, 2014). After these presentation we learned of the paper arXiv:1407.3232 who presented formula (5.31) for the case of $m = 1$ and $d = 2^{n'}$.

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