Achievable polarization for Heat-Bath Algorithmic Cooling

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Pure quantum states play a central role in applications of quantum information, both as initial states for many algorithms and as resources for quantum error correction. Preparation of highly pure states that satisfy the threshold for quantum error correction remains a challenge, not only for ensemble implementations like NMR or ESR but also for other technologies. Heat-Bath Algorithmic Cooling is a method to increase the purity of set of qubits coupled to a bath. We investigated the achievable polarization by analyzing the state when no more entropy can be extracted. In particular we give an analytic form for the maximum polarization of the purified qubit and corresponding state of the whole system for the case when the initial state of the qubits is totally mixed. It is however possible to reach higher polarization while starting with other states with higher polarization, thus our result provides an achievable lower bound. We also give an upper bound of the number of steps needed to get a certain required polarization.

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INTRODUCTION

Purification of quantum states is essential for the applications of quantum information science, not only for many quantum algorithms but also as a resource for quantum error correction. The need to find a scalable way to reach approximate pure states is a challenge for many modalities for quantum computations, especially for the ones that relies on ensembles such as NMR or ESR [1].

A potential solution is algorithmic cooling (AC), a protocol which purifies qubits by removing entropy of a subset of them, while increasing the entropy of others [2, 3]. An explicit way to implement this idea in ensemble quantum computers such as NMR was given by Schulman et al. [4]. They showed that it is possible to reach polarization of order unity using only a number of qubits which is polynomial in the initial polarization. This idea was improved by adding contact with a heat bath to extract entropy from the system [5], a process known as Heat Bath Algorithmic Cooling (HBAC). Based on this work, many practical cooling algorithms have been designed [6, 7, 8, 9, 10, 11]. Experiments have already demonstrated an improvement in polarization using this protocol with a few qubits [12–17], where a few rounds of HBAC were reached; and some studies have even included the impact of noise [13].

Through numerical simulations, Moussa [7] and Schulman et al. [8] observed that if the polarization of the bath ($\epsilon_b$) is much smaller than $2^{n-2}$, where $n$ is the number of qubits used, the asymptotic polarization reached will be $\sim 2^{n-2}\epsilon_b$; but when $\epsilon_b$ is greater than $2^{n-2}$, a polarization of order one can be reached. Inspired also by the work of Patange [19], who investigated the use of algorithmic cooling on spins bigger than $\frac{1}{2}$ (using NV center where the defect has an effective spin 1), we investigate the case of cooling a qubit using a spin $l$ in general, and an extra qubit that gets contact with the bath.

In this paper we give an analytic result for the asymptotic value of the polarization that can be reached if we start with the quantum computer in the totally mixed state coupled to a bath which has polarization $\epsilon_b$. This gives a lower bound to the achievable polarization as we can always efficiently turn a state into the maximally mixed one and some other initial states do lead to higher polarizations. We recover the limit of low polarization observed by Moussa and Schulman et al. also show how polarization of order one can be reached as a function of the number of qubits. We compare Schulman’s upper bound of the maximum probability of any basis state [10] with our analytical bound. Finally we give the number of rounds of compression/cooling needed to get certain polarization.

FIG. 1: HBAC can cool the spin−1/2 by compressing entropy into $m$ reset qubits and a $d$−dimensional spin−$l$ (or a string qubits of Hilbert space of dimension $d_f$); then, HBAC pumps entropy into a heat bath by refreshing the reset qubits.
HBAC technique purifies qubits by applying alternating rounds of entropy compression and pumping entropy into a thermal bath of partially polarized qubits, as explained below.

The system consists of a string of qubits: one qubit (a spin−1/2 also called the target) which is going to be cooled; one qubit (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 εm. Having the spin−l can be equivalent to having n′ qubits if the dimension of their Hilbert spaces is the same, i.e. if d = 2l + 1 = 2n′. We will also refer to the spin−1/2 and the spin−l as the computational qubits (Fig. 1).

The idea of the first step of HBAC is to re-distribute the entropy among the string of qubits applying an entropy compression operation U. This operation concentrates the entropy in the reset qubits of the system as much as possible by extracting entropy of the computational qubits. This process results in the cooling of the computational qubits while warming the reset qubits. The U needed makes a descending sort of the diagonal elements of the system’s density matrix.

The second step is to make use of the heat-bath for removing entropy. The m reset qubits are brought into thermal contact with the heat-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. We also assume that the heat bath has large heat capacity and the action of qubit-bath interaction on the bath temperature is negligible.

The total effect of applying these two steps on a system with state ρ can be expressed as follows:

\[ \rho \xrightarrow{\text{Compression}} \rho' = U \rho U^\dagger, \]
\[ \rho' \xrightarrow{\text{Refresh}} \rho'' = \text{tr}_{\text{m qubits}}(\rho') \otimes \rho_{\epsilon_m}^m, \]

where we assume U to be a permutation of the diagonal elements, \( \rho_{\epsilon_m} = \frac{1}{2} \begin{pmatrix} 1 + \epsilon_m & 0 \\ 0 & 1 - \epsilon_m \end{pmatrix} \), and \( \epsilon_m \) is the heat-bath polarization.

An interesting question is to know what is the asymptotic achievable cooling with this method, and how many iterations of the HBAC-steps would be needed to obtain a certain cooling, i.e. a certain value of polarization.

**COOLING LIMIT**

The cooling limit corresponds to the moment at which it is not possible to continue extracting entropy from the system, i.e. when the state of the computational qubits, \( \rho_{\text{com}} \), 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:

\[ \rho_{\text{com}} = \rho''_{\text{com}}, \]

where \( \rho_{\text{com}} = \text{tr}_{\text{n qubits}}(\rho) \). In general, the state of the qubit-system \( \rho \) can be expressed as follows:

\[ \text{diag}(\rho) = (p_1, p_2, ..., p_D), \]

where \( \text{diag}(\rho) \) is the vector of the diagonal elements of \( \rho \), and \( D = 2^{m+1}d \). Suppose that \( \rho \) corresponds to a state immediately after an entropy compression, its elements \( p_i \) will be sorted such that \( p_1 \geq p_2 \geq ... \geq p_D \).

The state of the computational qubits \( \rho_{\text{comp}} \) is given by tracing out the reset qubits out of the total state and is given by

\[ \text{diag}(\rho_{\text{comp}}) = (A_1, A_2, A_3, ..., A_{2d}). \]

The cooling limit will happen when we have the condition:

\[ A_i (1 - \epsilon_m)^m \geq A_{i+1} (1 + \epsilon_m)^m, \]

for \( i = 2, 3, ..., 2d - 1 \).

When this equation is satisfied, the entropy of the reset qubit 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 [3].

**MAXIMALLY MIXED INITIAL STATE**

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

\[ A_i (1 - \epsilon_m)^m \leq A_{i+1} (1 + \epsilon_m)^m, \]

where \( t \) labels the iteration step of HBAC. Obviously it is true for the initial step at \( t = 0 \) as all \( A_i \) are equal, 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 (the one to be cooled) never decreases and that the entropy of the reset qubits increases beyond the one from the bath and thus can be cooled by the bath before starting another round of compression.

Comparing eq.(6) and eq.(7) indicate that the asymptotic state of the computational qubit can only go towards the equality:

\[ A_i (1 - \epsilon_m)^m = A_{i+1} (1 + \epsilon_m)^m, \]

for all \( i = 2, 3, ..., 2d - 1 \).

From [8] and the property \( Tr(\rho_{\text{comp}}) = 1 \), it is possible to find \( A_i = \frac{1}{1 - \epsilon_m^2} Q^{i-2} \), where \( Q = \left( \frac{1 - \epsilon_m}{1 + \epsilon_m} \right)^m \). This result gives the exact solution of the steady state of the computational qubits, \( \tilde{\rho}_{\text{comp}} \) for all values of the bath polarization:

\[ \text{diag}(\tilde{\rho}_{\text{comp}}) = A_1 (1, Q, Q^2, ..., Q^{2d-1}). \]

The steady state of all the string will be

\[ \tilde{\rho} = \tilde{\rho}_{\text{comp}} \otimes \rho_{\epsilon_m}^m. \]
Asymptotic Polarization

From the steady state \((t \to \infty)\), eq. (9), the asymptotic polarization of the spin-1/2 is

\[
\epsilon_\infty^b = \frac{(1 + \epsilon_b)^{md} - (1 - \epsilon_b)^{md}}{(1 + \epsilon_b)^{md} + (1 - \epsilon_b)^{md}}. \tag{11}
\]

For the case of using a string of qubits instead of the scratch qubit, the maximum achievable polarization of the \(j\)th qubit will be \(\epsilon_{\max}^{(j)} = \frac{(1 + \epsilon_b)^{md} - (1 - \epsilon_b)^{md}}{(1 + \epsilon_b)^{md} + (1 - \epsilon_b)^{md}}\) (numbered from right to left on the string, Fig. [1]).

In the limit for low heat-bath polarization, \(\epsilon_b << 1/md\), the achievable asymptotic polarization is proportional to the dimension of the Hilbert space of the scratch qubit (or \(n'\) qubits), i.e. \(\epsilon_\infty^b \approx md\epsilon_b(= m2^n'\epsilon_b)\).

As the value of \(\epsilon_b\) increases beyond \(1/md\), we observe a transition for the asymptotic polarization. It is shown in Fig. [2] as a function of the heat bath polarization for different number of qubits, using eq. (11). We can observe the transition noted by [7] and [8] at \(\epsilon \approx 1/d\), agreeing with simulations. In order to see how \(\epsilon_\infty^b\) approaches 1, we use \(\Delta_{\max} = 1 - \epsilon_\infty^b\), and the eq. (11):

\[
\Delta_{\max} = \frac{2}{e^{md} \ln \left(\frac{1 + \epsilon_b}{1 - \epsilon_b}\right) + 1} = \frac{2}{e^{m2^n'} \ln \left(\frac{1 + \epsilon_b}{1 - \epsilon_b}\right) + 1}. \tag{12}
\]

This expression shows that the asymptotic polarization reaches 1 doubly exponentially in the number of qubits \(n'\) (or exponential as a function of the size of the Hilbert space \(d\)). In Fig. [2] we show \(\epsilon_\infty^b\) as a function of \(\epsilon_b\) for different values of \(d\), with \(m = 1\).

\[
\begin{array}{c|c|c|c|c|c|c|c|c}
\hline
\epsilon_\infty^b & d = 2 & d = 8 & d = 16 & d = 32 & d = 64 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 \\
0.1 & 0.09 & 0.04 & 0.01 & 0.00 & 0.00 \\
0.2 & 0.18 & 0.08 & 0.03 & 0.01 & 0.00 \\
0.3 & 0.27 & 0.12 & 0.05 & 0.01 & 0.00 \\
0.4 & 0.37 & 0.18 & 0.07 & 0.02 & 0.00 \\
0.5 & 0.47 & 0.24 & 0.09 & 0.03 & 0.00 \\
0.6 & 0.57 & 0.30 & 0.11 & 0.04 & 0.00 \\
0.7 & 0.67 & 0.36 & 0.13 & 0.05 & 0.00 \\
0.8 & 0.77 & 0.41 & 0.15 & 0.06 & 0.00 \\
0.9 & 0.87 & 0.46 & 0.17 & 0.07 & 0.00 \\
1 & 1 & 1 & 1 & 1 & 1 \\
\hline
\end{array}
\]

FIG. 2: Asymptotic achievable polarization for the target qubit. That polarization increases double exponentially in the number of computational qubits \(n'\). The dot represents the point when \(\epsilon_\infty^b = 1/d\), where the transition can be observed, for \(n' = 1, 2, 3, 4, 5, \text{and} 6\).

The asymptotic polarization \(\epsilon_\infty^b\) 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 but nevertheless obeys eq. (7). Numerical simulation indicates that this could also happen with some initial states not obeying eq. (7). But we also can find explicit examples of initial states that lead to asymptotic polarizations that are higher than eq. (11). As any state can be efficiently maximally randomized, it is always possible to reach the polarization given eq. (11) and maybe do better if the initial state is different.

Schulman’s Physical-Limit Theorem

The steady state, eq. (9), is consistent with the fundamental limits of HBAC given by the theorem of Schulman et al. [10]. 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 say more than \(\min\{2^{-n}e^{2n-1}, 1\}\). Where \(\epsilon\) is related to the polarization of the heat bath as \(\epsilon_b = \tanh\frac{\epsilon}{2}\), and \(n\) is the total number of qubits \((n = n' + 1: \text{n’ computational qubits and one reset qubit})\).

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: \(p_{\max} = A_1(1 + \epsilon_b)/2\) (from eq. (9) and [10]). That expression can by written as a function of \(n\) and \(\epsilon_b\) as follows: \(p_{\max} = \frac{\epsilon_b}{1 - (\frac{1 + \epsilon_b}{1 - \epsilon_b})^{2n-1}}\).

Fig. 3 shows the upper bound proposed by Schulman (dashed lines) and the asymptotic value obtained here (thick lines), for different values of \(n\). We can see for small values of \(\epsilon_b\) that the upper limit of them is very close to the exact solution, but differ for large values of \(\epsilon_b\).
We evaluate the number of steps required to get a certain polarization for the case of using a three qubits string (n=1, d=2). For this, we need to know how the polarization evolves after applying the steps of the HBAC method. For the case of three qubits initially in a total mixed state, the quantum circuit required to perform optimally the HBAC method is known, see Fig. 4.

![Quantum circuit for HBAC method on a system of three qubits starting in total mixed state.](Image)

**FIG. 4:** Quantum circuit for HBAC 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 refreshing plus one compression), subsequent iterations are just the repetition of the iterations 1 and 2 (a 3q-Round).

Consider that the polarization of the first qubit is $\epsilon'$. After applying the two corresponding operations to the 3q-Round in Fig. 4, the polarization of the target qubit increases from $\epsilon'$ to $\epsilon'^{t+2}$ as follows:

$$\epsilon'^{t+2} = 2abe^t + \epsilon_b,$$

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

Let $t=0$ after the first iteration, then $\epsilon^0 = \epsilon_b$. From eq. (13), we have that the polarization after apply $j$ times the two steps, can be written as follows:

$$\epsilon^{t=2j} = \epsilon_1^\infty - q^{t} (\epsilon_1^\infty - \epsilon_b).$$

where $q = \frac{1 - \epsilon_b^2}{2}$. Using (11), we have that the asymptotic polarization for $d = 2$ is $\epsilon_1^\infty = \frac{2\epsilon_b}{1 + \epsilon_b}$. From this equation we can find the number of steps needed to get $\epsilon = \epsilon_1^\infty - \delta$, as function of $\epsilon_1^\infty$ and $\delta$.

$$N(\delta, \epsilon_b) = 2j = 2 \frac{\log \left( \frac{\delta}{\epsilon_1^\infty - \epsilon_b} \right)}{\log q}. \quad (15)$$

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

$$N_{\text{upper-bound}} = \prod_{k=1}^{k=[n'/2]} N(\delta_k, \epsilon_k), \quad (16)$$

where $\epsilon_{\text{max}} = \frac{(1+\epsilon_b)^{d/2} - (1-\epsilon_b)^{d/2}}{(1+\epsilon_b)^{d/2} + (1-\epsilon_b)^{d/2}}$; $\epsilon_k = f(\epsilon_{k-1}) - \delta_k$; $\epsilon_{h, \delta} = \epsilon_h$, with $h = [n'/2]$ (the integer part of $n'/2$); $f(\epsilon) = \frac{2\epsilon}{1+\epsilon} N(\delta, \epsilon) = 2 \frac{\log \left( \frac{\delta}{\epsilon_1^\infty - \epsilon_b} \right)}{\log q}$; and $\epsilon_0 = \epsilon_b$.

**CONCLUSION**

HBAC is a process to purify a number of qubits using extra qubits and contact with a bath. We presented an analytical solution for the steady state which corresponds to the cooling limit of a string of qubits starting with the totally mixed state which consists of one qubit with a number of ancilla qubits (or a spin-l) and another set of $m$ qubits that can be put into contact with a bath with polarization $\epsilon_b$. From this formula we can understand the transition of behavior of the asymptotic polarization at $1/md$. Below this value, $\epsilon_1^\infty \sim m d \epsilon_b$ and above it will reach order unity double exponentially with the number of scratch qubits. This behavior will remain true for other initial states as long as they obey conditions (7). We can think of our derived asymptotic polarization as the minimum polarization limit as it is always possible to efficiently randomized a state so that value can always be reached. If conditions (7) are not obeyed, it is possible (but not necessary) to reach higher polarization. Finally, we have also use the formula obtained to derive the number of steps required to reach a given polarization for a specific number of qubits [20].
SUPPLEMENTAL MATERIAL

Here we explain how to obtain the maximum achievable polarization of heat bath algorithmic cooling (HBAC), starting with the totally mixed state. First we give the conditions to have a steady state. Then we show that starting with the maximally mixed state, can reach these conditions only asymptotically. From this asymptotic state we derive the maximum polarization achievable, again starting from the maximally mixed state. We also explain how to get the number of steps needed to have a certain polarization $\epsilon_{\text{max}} - \delta$ (we give the exact solution for $n = 3$ and upper bound for $n > 3$).

COOLING LIMIT

The state at the cooling limit corresponds to the one where it is not possible to continue extracting entropy of the system, i.e. when the state of the system does not change by the compression and refresh steps.

The plan to find this steady state is to consider a general form of $\rho$ and apply the two steps of the HBAC method to get $\rho''$. Equality to the two states give the conditions for the steady state. We assume that the density matrix is diagonal. By applying compression (permutations) and refresh operations the state remains diagonal. Thus the state can be completely described by its diagonal elements,

$$\text{diag}(\rho) = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_D \end{bmatrix},$$

where $\text{diag}(\rho)$ is the vector of the diagonal elements of $\rho$, 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:** $\rho \xrightarrow{\text{Compress}} \rho' = U \rho U^\dagger$, where $U$ sorts the diagonal elements of $\rho'$ in decreasing order:

$$p_1' \geq p_2' \geq \ldots \geq p_D' \geq p_D.'$$

**Refresh Step:** $\rho' \xrightarrow{\text{Refresh}} \rho'' = \text{tr}_m(\rho') \otimes \rho_m^{\otimes m}$, where $\text{tr}_m()$ is the partial trace operation over the m reset qubits, and $\rho_m = \frac{1}{2} \begin{pmatrix} 1 + \epsilon_b & 0 \\ 0 & 1 - \epsilon_b \end{pmatrix}$ represents a qubit with heat bath polarization $\epsilon_b$. We define $\rho_{\text{comp}} = \text{tr}_m(\rho')$, the state of the computational qubits, and is

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[1] T. D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe, and J. L. O’Brien, Nature 464, 45 (2010) and arXiv:1009.2267.
[2] O. W. Sørensen, Journal of Magnetic Resonance (1990) 86, 435 (1990).
[3] O. W. Sørensen, Journal of Magnetic Resonance (1969) 93, 648 (1991).
[4] L. J. Schulman and U. Vazirani, in Proceedings of the 31st Annual ACM Symposium on the Theory of Computation (STOC) (ACM Press, El Paso, Texas, 1998) pp. 322–329.
[5] P. O. Boykin, T. Mor, V. Roychowdhury, F. Vatan, and R. Vrijen, Proceedings of the National Academy of Sciences 99, 3388 (2002).
[6] J. M. Fernandez, S. Lloyd, T. Mor, and V. Roychowdhury, International Journal of Quantum Information 2, 461 (2004).
[7] O. Moussa, On heat-bath algorithmic cooling and its implementation in solid-state NMR, Master of science in physics thesis, University of Waterloo (2005).
[8] L. Schulman, T. Mor, and Y. Weinstein, Physical review letters 94, 120501 (2005).
[9] Y. Elias, J. M. Fernandez, T. Mor, and Y. Weinstein, Israel Journal of Chemistry 46, 371 (2006).
[10] L. J. Schulman, T. Mor, and Y. Weinstein, SIAM Journal on Computing 36, 1729 (2007).
[11] Y. Elias, T. Mor, and Y. Weinstein, Physical Review A 83, 042340 (2011).
[12] J. M. Fernandez, T. Mor, and Y. Weinstein, International Journal of Quantum Information 3, 281 (2005).
[13] J. Baugh, O. Moussa, C. A. Ryan, A. Nayak, and R. Laflamme, Nature 438, 470 (2005).
[14] C. A. Ryan, O. bMoussa, J. Baugh, and R. Laflamme, Phys. Rev. Lett. 100, 140501 (2008).
[15] Y. Elias, H. Gilboa, T. Mor, and Y. Weinstein, Chemical Physics Letters 517, 126 (2011).
[16] G. Brassard, Y. Elias, J. M. F. N. H. Gilboa, J. A. Jones, T. Mor, Y. Weinstein, and L. Xiao, (2014, arXiv:1404.6885).
[17] G. Brassard, Y. Elias, T. Mor, and Y. Weinstein, arXiv preprint arXiv:1404.6824 (2014).
[18] P. Kaye, Quantum Information Processing 6 (2007).
[19] O. Patange, On an Instrument for the Coherent Investigation of Nitrogen-Vacancy Centres in Diamond, Master of science in physics thesis, University of Waterloo (2013).
[20] This work was presented on a poster at the Institute for Quantum Computing (March 27, 2014) and at the 14th Annual Canadian Summer School on Quantum Information at the Univ. of Guelph (June 16-20, 2014). After these events we learned of the paper arXiv:1407.3232 who showed formula (11) for the case of $d = 2^m$ & $m = 1$.
Let \( A_i^t \) be the evolution of \( A_i \) after \( t \) iterations of HBAC, with \( A_i^0 := A_i \). Interestingly, if we start with the totally mixed state with have

\[
A_i^0(1 - \epsilon_b) \leq A_i^0(1 + \epsilon_b),
\]

for all \( i = 1, 2, \ldots, 2d - 1 \) and note that it is a less than equal sign in distinction from (23). We will show that if (24) is true at \( t = 0 \) it will be true for all future steps \( t \). Moreover we will also show that if (24) is obeyed, the rounds of HBAC keep cooling the computational qubits. Thus the state of the system reaches asymptotically the condition of (23) with the equality.

Now we are going to prove that if we have \( A_i^t \leq \frac{1 + \epsilon_b}{1 - \epsilon_b} \) for all \( i = 1, 2, \ldots, 2d - 1 \), at a given time, then after an iteration of HBAC we will also have \( A_i^{t+1} \leq \frac{1 + \epsilon_b}{1 - \epsilon_b} \).

Let \( \rho_i^{t+1} \) be the state of the computational qubits after \( t \) iterations. Then, the density matrix of the total state will be given by \( \rho_t = \rho_i^{t+1} \otimes \rho_{\text{reset}} \), with refreshed reset qubit. Thus, the total state is as follows:

\[
\begin{bmatrix}
A_1^t (1 + \epsilon_b) \\
A_2^t (1 - \epsilon_b) \\
\vdots \\
A_{2d}^t (1 + \epsilon_b) \\
A_{2d}^t (1 - \epsilon_b)
\end{bmatrix}
\]

In general, the elements of \( \rho_t \) can be written as

\[
p_{2i-1}^t = A_i^t(1 + \epsilon_b)/2, \quad p_{2i}^t = A_i^t(1 - \epsilon_b)/2,
\]

for \( i = 1, 2, \ldots, 2d \).

Now, we have to compress \( \rho_t \) to get \( \rho_t^{t+1} \), i.e. we have to sort the elements of \( \text{diag}(\rho_t) \) in decreasing order.

Observe that the elements with factor \( 1 + \epsilon_b \) (blue elements in (25)) are already in descending order, since \( A_1^t \geq A_2^t \geq \ldots \geq A_{2d}^t \). Therefore, during the compression step, even these elements will be moved to different entries of the diagonal matrix from the initial ones, they will have the same order. Similarly for the elements with factor \( 1 - \epsilon_b \) (red elements).

Assuming \( \frac{A_i^t}{A_{i+1}^t} \leq \frac{1 + \epsilon_b}{1 - \epsilon_b} \), it 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 \( A_{2d}^t(1 - \epsilon_b) \) which stays in the same position.
Considering this movement of the elements, we can conclude that the elements of \( \rho_{t+1} \) will satisfy the following:

\[
A_i^t(1 - \epsilon_b) \leq p_{2t+1}^{(t+1)} \leq A_i^t(1 + \epsilon_b), \quad (28)
\]

\[
A_i^t(1 - \epsilon_b) \leq p_{2t+1}^{(t+1)} \leq A_i^{t+1}(1 + \epsilon_b), \quad (29)
\]

for \( i = 2, 3, ..., 2d - 1 \).

The new computational state, \( \rho_{t+1}^{\text{comp}} = \text{tr}(\rho^{t+1}) \), will have diagonal elements \( A_i^{t+1} = p_{2t+1}^{(t+1)} + p_{2t}^{(t+1)} \), from this and \( (28)-(29) \),

\[
(A_i^{t+1} + A_i^t)(1 - \epsilon_b) \leq A_i^{t+1}(1 + \epsilon_b) \leq (A_i^t + A_i^{t+1})(1 + \epsilon_b), \quad (30)
\]

for \( i = 2, 3, ..., 2d - 1 \). For \( i = 1 \) and \( i = 2d \), we know exactly the corresponding diagonal elements,

\[
A_1^{t+1} = (A_1^t + A_2^t)(1 + \epsilon_b)/2, \quad (31)
\]

\[
A_{2d}^{t+1} = (A_{2d-1}^t + A_{2d}^t)(1 - \epsilon_b)/2. \quad (32)
\]

These last three equations imply that \( A_i^{t+1} \) satisfy the following inequality:

\[
\frac{A_i^{t+1}}{A_i^{t+1} + 1} \leq \frac{A_i^t(1 + \epsilon_b) + A_i^{t+1}(1 + \epsilon_b)}{A_i^t(1 - \epsilon_b) + A_i^{t+1}(1 - \epsilon_b)} = \frac{1 + \epsilon_b}{1 - \epsilon_b}, \quad (33)
\]

for all \( i = 1, 2, ..., 2d - 1 \), as we claimed.

**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 \( (23) \). To show this, we will prove that the target qubit (the spin−1/2) is cooled after each iteration of HBAC, and the rest 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.\((25)\), when the reset qubit is already refreshed). Then, the reduced density matrix for the target qubit is

\[
\text{diag}(\rho_{t}^{\text{target}}) = \begin{bmatrix} \rho_{00,\text{target}}^t \\ \rho_{11,\text{target}}^t \end{bmatrix}, \quad (34)
\]

where \( \rho_{00,\text{target}}^t = \sum_{i=1}^{2d} p_i^t = \sum_{i=1}^{d} A_i^t \), and \( \rho_{11,\text{target}}^t = 1 - \rho_{00,\text{target}}^t \).

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

\[
\implies \rho_{00,\text{target}}^t \geq \rho_{00,\text{target}}^{t+1}, \quad (35)
\]

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 \( \rho_r^t \) when the total system has state \( \rho^t \). Then,

\[
\text{diag}(\rho_r^{t+1}) = \begin{bmatrix} \rho_{00,\text{target}}^{t+1} \\ \rho_{11,\text{target}}^{t+1} \end{bmatrix}, \quad (36)
\]

where \( \rho_{00,\text{target}}^t = \sum_{i=1}^{2d} p_i^{t+1} \). This equation with \( (28) \) and \( (26) \) gives

\[
\rho_{00,\text{target}}^{t+1} = \sum_{i=1}^{2d} p_i^{t+1} \leq \sum_{i=1}^{2d} A_i^t(1 + \epsilon_b)/2 = (1 + \epsilon_b)/2. \quad (37)
\]

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 with implies that the reset qubit always extracts entropy from the system when it is brought into contact with the heat bath, cooling the total system in every iteration, unless it is in the cooling limit.

The two elements above show that, starting from the totally mixed state, we will converge to the equality of \( (23) \). At this limit the steady state of the computational qubits should have elements which satisfy

\[
\frac{A_i^\infty}{A_i^{t+1}} = \frac{1 - \epsilon_b}{1 + \epsilon_b} \equiv Q. \quad (38)
\]

Using eq.\((38)\) and \( \text{Tr}(\rho_{\text{comp}}) = 1 \), it is possible to find the exact solution of each \( A_i^\infty \),

\[
A_i^\infty = \frac{1 - Q}{1 - Q^{2d}Q^{-2}}, \quad (39)
\]

and therefore the analytical solution of the steady state of the computational qubits, \( \rho_{\text{comp}}^\infty \):

\[
\text{diag} (\rho_{\text{comp}}^\infty) = A_1^\infty \begin{bmatrix} 1 \\ Q \\ Q^2 \\ \vdots \\ \vdots \\ Q^{2d-1} \end{bmatrix}. \quad (40)
\]

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

Using eq.\((40)\), the reduced density matrix of the target qubit in the cooling limit, is given by:

\[
\text{diag}(\rho_{\text{target}}^\infty) = A_1^\infty \sum_{i=0}^{d-1} Q^i \begin{bmatrix} 1 \\ Q^i \\ \frac{1}{2} \left[ 1 + \epsilon_b^\infty \right] \end{bmatrix}. \quad (41)
\]
where $\epsilon_1^\infty$ is the asymptotic polarization of the target qubit when we start with the maximally mixed state.

From this equation we can derive:

$$
\epsilon_1^\infty = \frac{(1 + \epsilon_b)^d - (1 - \epsilon_b)^d}{(1 + \epsilon_b)^d + (1 - \epsilon_b)^d},
$$

(42)

where $d$ is the dimension of the Hilbert space of the total system of scratch qubit ($d = 2^{l+1}$ 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 given by

$$
\rho_{\epsilon_b}^{\otimes m} = \left(1 + \epsilon\right)^{\otimes m}_{\epsilon} = \begin{pmatrix}
(1 + \epsilon)^m \\
. \\
. \\
(1 - \epsilon)^m
\end{pmatrix},
$$

(43)

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. (21), $\rho''$ is as follows:

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

First notice that any swap between two elements from 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, they will contribute to the sum of the probabilities corresponding to same basis state of the computational qubits that they contributed before the compression, which does not make any improvement on the computational state entropy compression.

Then, we are just interested in permuting elements to a different box from where they were originally, in particular the biggest element or smallest element of each box (to have the maximum entropy compression). In 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:

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

(44)

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

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

(45)

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

$$
diag (\rho_{\text{comp}}^{\infty}) = A_1^\infty \begin{pmatrix}
1 \\
Q_m \\
. \\
. \\
. \\
Q^{(2d-1)m}
\end{pmatrix}
$$

(46)

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

$$
\epsilon_1^\infty = \frac{(1 + \epsilon_b)^{md} - (1 - \epsilon_b)^{md}}{(1 + \epsilon_b)^{md} + (1 - \epsilon_b)^{md}}.
$$

(47)

Note that a similar polarization would be obtained if we start with a different initial state but which obeys eq. (24). Numerical simulation indicate that this could also happens with some initial states not obeying eq. (24). And finally we can give explicit example of initial states that lead to an asymptotic polarization that are higher than eq. (47).

**Polarization of different computational qubits**

Consider the case of having a string of $n'$ qubits as scratch qubits. 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 of the qubits from the steady state \( |0\rangle \). 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

\[
\text{diag}(\rho^\infty_{\text{target}}) = \text{tr}_{\text{target}}(\rho^\infty_{\text{comp}}) = \begin{bmatrix}
A_1^\infty + A_{d+1}^\infty \\
A_2^\infty + A_{d+2}^\infty \\
\vdots \\
A_d^\infty + A_{2d}^\infty
\end{bmatrix}. \tag{48}
\]

Let \( B_i \) be the \( i \)th element of \( \text{diag}(\rho^\infty_{\text{target}}) \), i.e. \( B_i = A_i^\infty + A_{d+i}^\infty \). From eq. \( 39 \), \( B_i = A_i^\infty Q^{i-1} + A_{d+i}^\infty Q^d = A_i^\infty (1 + Q^{d-1})Q^{-1} \). Thus, \( B_i = kQ^i \), where \( k = A_i^\infty (1 + Q^d)Q \). Comparing \( B_i \) with eq. \( 39 \), we see that this state has the same form of the state eq. \( 40 \), but with Hilbert space dimension \( d/2 \). Thus, the asymptotic polarization of the \( n \)th qubit is

\[
\epsilon^{(n')}_{\text{max}} = \frac{(1 + \epsilon_b)^{md/2} - (1 - \epsilon_b)^{md/2}}{(1 + \epsilon_b)^{md/2} + (1 - \epsilon_b)^{md/2}} \tag{49}
\]

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

\[
\epsilon^{(j)}_{\text{max}} = \frac{(1 + \epsilon_b)^{m2^{j-1}} - (1 - \epsilon_b)^{m2^{j-1}}}{(1 + \epsilon_b)^{m2^{j-1}} + (1 - \epsilon_b)^{m2^{j-1}}}. \tag{50}
\]

**Number of Steps Needed to get \( \epsilon = \epsilon_4^\infty - \delta \)**

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

The quantum circuit required to perform the HBAC on three qubits initially in the total mixed state is shown in Fig. \( 4 \). 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 the Fig. \( 4 \). The application of those two iterations will be referred as a 3q-Round.

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

\[
\text{diag}(\rho^t_{\text{comp}}) = \begin{bmatrix}
A_1^t \\
A_2^t \\
A_3^t \\
A_4^t
\end{bmatrix}, \tag{51}
\]

and the total system as \( \rho' = \rho^t_{\text{comp}} \otimes \rho_A \). The polarization of the target qubit, \( \epsilon^t \), can be obtained from its reduced density matrix, \( \text{diag}(\rho^t_{\text{target}}) = \begin{bmatrix}
A_1^t + A_2^t \\
A_3^t + A_4^t
\end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + \epsilon^t \end{bmatrix} \)

\[ \implies \epsilon^t = 2(A_1^t + A_2^t) - 1. \tag{52} \]

In the first iteration of the 3q-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. \( 6 \) thus

\[
\begin{bmatrix}
A_1^t (1 + \epsilon_b) \\
A_1^t (1 - \epsilon_b) \\
A_2^t (1 + \epsilon_b) \\
A_2^t (1 - \epsilon_b)
\end{bmatrix} \implies \frac{1}{2} \begin{bmatrix}
A_1^t (1 + \epsilon_b) \\
A_1^t (1 - \epsilon_b) \\
A_2^t (1 + \epsilon_b) \\
A_2^t (1 - \epsilon_b)
\end{bmatrix}. \tag{53}
\]

Then, the density matrix of the computational qubits after the first iteration of the 3q-Round is

\[
\text{diag}(\rho^{t+1}_{\text{comp}}) = \frac{1}{2} \begin{bmatrix}
(A_1^t + A_2^t) (1 + \epsilon_b) \\
(A_1^t + A_2^t) (1 - \epsilon_b) \\
(A_3^t + A_4^t) (1 + \epsilon_b) \\
(A_3^t + A_4^t) (1 - \epsilon_b)
\end{bmatrix} \tag{54}
\]

In the second iteration of the 3q-Round, the compression step is performed by applying the unitary matrix shown in Fig. \( 7 \). In this step we obtain \( \rho^{t+2} \):

\[
\begin{bmatrix}
(A_1^t + A_2^t) (1 + \epsilon_b) \\
(A_1^t + A_2^t) (1 - \epsilon_b) \\
(A_3^t + A_4^t) (1 + \epsilon_b) \\
(A_3^t + A_4^t) (1 - \epsilon_b)
\end{bmatrix} \tag{55}
\]

From this state, with the normalization property of the density matrix and eq. \( 52 \), we can obtain the new polarization of the target qubit,

\[
\epsilon^{t+2} = 2ab\epsilon^t + \epsilon_b, \tag{56}
\]

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. \( 4 \)), then the polarization of the target qubit at that moment will be \( \epsilon^0 = \epsilon_b \). Then, from eq. \( 54 \), we can get the exact polarization after each 3q-Round, i.e. every two iterations,

\[
\epsilon^{t+2j} = \frac{2\epsilon_b}{1 + \epsilon_b} - q^{2j} \left( \frac{2\epsilon_b}{1 + \epsilon_b} - \epsilon_0 \right), \tag{57}
\]

where \( q = 1 - \frac{\epsilon_2}{\epsilon_b} \). From eq. \( 47 \), the asymptotic polarization for this case is \( \epsilon^\infty_4 = \frac{2\epsilon_b}{1 + \epsilon_b} \), thus the equation \( 55 \) can be written as

\[
\epsilon^{t+2j} = \epsilon^\infty_4 - q^{2j} (\epsilon_{\text{max}} - \epsilon_0). \tag{58}
\]
Since $q < 1$, $\epsilon^j \to \epsilon^\infty$ when we increase $j$.

We can use (56) to know the number of steps $t$ needed to achieve polarization $\epsilon^\infty - \delta$. From Eq. (56), we have $\delta = q^j (\epsilon_{\text{max}} - \epsilon_b)$, then the number of required steps $N$ will be

$$N(\delta, \epsilon_b) := t = 2 \frac{\log \left( \frac{\delta}{\epsilon^\infty - \epsilon_b} \right)}{\log q}.$$  \hspace{1cm} (57)

to get polarization

$$\epsilon_\delta(\epsilon_b, \delta) := \epsilon^\infty - \delta = \frac{2\epsilon_b}{1 + \epsilon_b^2} - \delta.$$ \hspace{1cm} (58)

**Numerical results**

Let $\delta_{\text{rel}} = \frac{\epsilon^\infty - \epsilon}{\epsilon^\infty} = \hat{\delta}$. Fig. 5 shows the number of refresh steps needed to achieve a polarization $\epsilon = \epsilon^\infty (1 - \delta_{\text{rel}})$ as function of $\delta_{\text{rel}}$ for different values of $d$.

We already have the exact solution of number of steps needed for the case of $d=2$ and one reset qubit, i.e. 3 qubits in the string, which is consistent with the results from the simulations.

**Upper bound of the number of steps to get a certain polarization $\epsilon$, for n qubits**

Consider a string of $n' = n - 1$ 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 number 1 to cool the qubit number 2, we can increase the polarization of the qubit number 2 to $\epsilon_1 = \epsilon_{\delta}(\epsilon_b, \delta)$ in $N_1 = N(\delta, \epsilon_b)$ steps, from (57) and (58).

After this preparation of the qubit 2, we can swap it with qubit 3, and then prepare again the qubit 2. We can apply again the compression for three qubits, but now using the 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 the 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, this number of iterations gives an upper bound of the number of steps to achieve polarization $\epsilon < \epsilon_{\text{max}}$ on the target qubit, where $\epsilon_{\text{max}} = \epsilon^\infty = \frac{(1+\epsilon_b)^d/2 - (1-\epsilon_b)^d/2}{(1+\epsilon_b)^d/2 + (1-\epsilon_b)^d/2}$, and $\epsilon = \epsilon_{\delta}(\epsilon_{h-1}, \delta)$ with $\epsilon_0 = \epsilon_b$, and $h = \lceil n'/2 \rceil$ (the integer part of $n'/2$). The upper bound is $N_{\text{upper-bound}} = \prod_{k=1}^{h} N(\delta, \epsilon_k).$
FIG. 6: Matrix and circuit symbol corresponding to the entropy compression step of the iteration 1. This gate swaps the scratch qubit and the reset qubit.

FIG. 7: Matrix and circuit symbol corresponding to the entropy compression of the iteration 2.