The Asymptotic Cooling of Heat-Bath Algorithmic Cooling

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The purity of quantum states is a key requirement for many quantum applications [1–3]. Improving the purity is limited by fundamental laws of thermodynamics [5, 6]. Here we are probing the fundamental limits for a natural approach to this problem, namely heat-bath algorithmic cooling (HBAC). The existence of the cooling limit for HBAC techniques was proved by Schulman et al. in [7], the limit however remained unknown for the past decade [7, 19, 23, 25]. Here for the first time we find this limit. In the context of quantum thermodynamics, this corresponds to the maximum extractable work from the quantum system.

The purity of quantum states is a key requirement for many quantum applications [1–3]. Improving the purity is limited by fundamental laws of thermodynamics [5, 6]. Here we are probing the fundamental limits for a natural approach to this problem, namely heat-bath algorithmic cooling (HBAC). The existence of the cooling limit for HBAC techniques was proved by Schulman et al. in [7], the limit however remained unknown for the past decade [7, 19, 23, 25]. Here for the first time we find this limit. In the context of quantum thermodynamics, this corresponds to the maximum extractable work from the quantum system.

Here we consider a quantum system that is in interaction with a heat-bath. The quantum system comprises two kind of qubits, the computation qubits and the reset qubits. The computation qubits are the high quality qubits with long decoherence time that are used for computation. The reset qubits on the other hand have shorter relaxation time and equilibrate fast. We assume that the equilibrium state is \( \rho_{eq} = e^{-\beta H} \), where \( \beta = \frac{1}{KB} \) with \( K_b \) the Boltzmann factor and \( T \) the temperature. Figure 1 shows a schematic of the model that we are considering in our work.

This model applies to a variety of physical systems. For instance, in NMR, the system is the few nuclear spins that can be controlled and other magnetic moments in the sample make the heat-bath. These magnetic moments couple to the nuclear spins in the system and eventually equilibrate them. Different spin species have different coupling rates [7, 18].

The class of cooling transformations that we are considering here are known as heat-bath algorithmic cooling [7, 13, 26]. HBAC is a quantum computation technique for cooling computation qubits by transferring their entropy to the reset qubits. The reset qubits are regularly refreshed through their interaction with the heat-bath.

The original idea of algorithmic cooling was developed by Schulman and Vazirani in [27] which uses a technique for Schumacher’s quantum data compression [28, 29]. Later it was proposed to use a heat-bath to enhance the cooling beyond the compression bounds [26, 30]. The idea is that after the entropy transfer, the heat-bath refreshes the hot qubits and then the entropy transfer can be repeated. Different iterative methods were developed based on this idea [23, 24, 29]. All of these methods are referred to as “Heat-Bath Algorithmic Cooling”.

As mentioned above, it is not possible to extract all the entropy of the computation qubits and cool them down arbitrarily [7], but the actual HBAC cooling limit remained unknown for almost ten years.

In this work, we find the cooling limit for HBAC. We find the asymptotic state of the computation and reset qubits which gives the cooling limit of the qubits in this framework. This fundamental limit sets the ultimate
Computation Qubits
Heat-Bath
Reset Qubits

Figure 1: The schematic of the model. The quantum system comprises computation qubits and reset qubits and interacts with a heat-bath. The heat-bath incorporates degrees of freedom in the environment that couple to the qubits in the quantum system. Usually, different qubits couple differently to these degrees of freedom. The computation and the reset qubits interact respectively weekly and strongly with the heat-bath. We ignore the weak interaction between the computation qubits and the heat-bath and assume that only the reset qubits are effected by the interaction with the heat-bath. The goal is to cool down the qubits in the system. Note that this is just a schematic and in reality they are not necessarily spatially arranged in this way. The HBAC does not cool all the qubits to the same temperature and the asymptotic temperature of different computation qubits would be different.

We focus on the coolest qubit and find its asymptotic state. We then calculate its temperature which is the cooling limit for all the HBAC techniques.

limit of any practical cooling approach under similar constraints.

We use the technique that was introduced in [7]. It is called the “Partner Pairing Algorithm (PPA)” and is the optimal technique for HBAC. We find the cooling limit for the PPA and as it is the optimal technique, the limit applies to all the HBAC techniques as well.

The PPA is an iterative method. In each iteration, the diagonal elements of the density matrix are sorted and then the reset qubit is refreshed. The reset process is equivalent to

\[ R(\rho) = \text{Tr}_R(\rho) \otimes \rho_R. \]  \hspace{1cm} (1)

\( \text{Tr}_R(\cdot) \) is the partial trace over the reset qubit and \( \rho_R = \frac{1}{e^{-\epsilon}+e^{\epsilon}} \begin{pmatrix} e^\epsilon & 0 \\ 0 & e^{-\epsilon} \end{pmatrix} \), is the fixed point of the reset process which is the equilibrium state. The parameter \( \epsilon \) is called the polarization and \( \epsilon = \frac{\Delta}{2 K_b T_B} \), where \( \Delta \) is the energy gap of the reset qubit, \( K_b \) is the Boltzmann constant, and \( T_B \) is the temperature of the heat-bath. Polarization is commonly used to quantify the purity of spins. The higher the polarization, the purer and colder the qubit is.

For a qubit with the state \( \rho = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \) the polarization is given by \( \frac{1}{2} \log \left( \frac{2}{a^2+b^2} \right) \).

The reset step cools down the reset qubit and changes the diagonal elements of the density matrix which also changes their ordering. The sort operation in the following iteration would then increase the polarization of computation qubits. Figure 2 shows the procedure of each iteration.

Despite the simplicity of each iteration, the dynamics are complicated and it is difficult to understand how the state evolves under these dynamics. In particular, it is challenging to find the asymptotic state that the process converges to [23, 24].

We take a different approach for finding the cooling limit. Instead of focusing on the dynamics, we note that the state of the system iteratively undergoing the HBAC algorithm will converge to an asymptotic state which is a fixed point of the HBAC procedure, and thus focus on the properties of this asymptotic state.

We use \( \rho_i = \{ \lambda_1^{(i)}, \lambda_2^{(i)}, \cdots, \lambda_n^{(i)} \} \) to show the state of \( n \) computation qubits plus one reset qubit which is the last one. The superscript represents the iteration index and the subscript is the index of the diagonal elements.

HBAC cools the first qubit monotonically which means that we just need to find the asymptotic state \( \rho_\infty \) to find the cooling limit. This state does not change under the operations of HBAC and is the fixed point of the dynamics. This leads to the following condition for the asymptotic state:

\[ p_i^\infty e^{-\epsilon} = p_{i+1}^\infty e^{\epsilon}, \forall i, \]  \hspace{1cm} (2)

where \( p_i \) are the diagonal elements of the density matrix of computation qubits.

This condition together with the normalization of the state is enough to determine the full state. Equation (2) can be rewritten as \( p_i^\infty = e^{-2\epsilon} p_0^\infty \) and considering state normalization gives:

\[ p_0^\infty = \frac{e^{-2\epsilon}-1}{(e^{-2\epsilon})^2-1}. \]  \hspace{1cm} (3)

Schulman et al. upper bounded \( p_0^\infty \) by \( \frac{e^{2n+\epsilon}}{2} \) in [7] which is consistent with our result. Figure 3 gives a comparison between this bound and the actual value from equation (3). Plots are for \( n = 2 \) and one reset qubit. Figure 3
Figure 3: Comparison of the upper bound and value of $P_0^\infty$. The gap between the upper bound and the actual value gets larger as $\epsilon$, the polarization of the reset qubit increases.

Equations (2) and (3) give the asymptotic state $[\rho^\infty] = P_0^\infty \{ 1, e^{-2\epsilon}, e^{-4\epsilon}, \ldots \} \otimes \rho_R$.

The first qubit has the lowest temperature. Therefore, we focus on the first computation qubit for finding the cooling limit. We find that the polarization of the first qubit is

$$P = 2^{n-1} \epsilon.$$ (4)

This result is consistent with the lower bound that was calculated under the assumption that $\epsilon \ll \frac{1}{2D}$ in [23].

Equation (4) shows that the performance of HBAC increases exponentially with the number of qubits, $n$. The simple way to see this is to look at the effective temperature. The effective temperature of the first qubit is

$$T_{\text{eff}} = \frac{\delta}{\Delta} T_{B} \frac{2^n-1}{\epsilon},$$ (5)

where $\delta$ is the energy gap of the qubit is often different from $\Delta$, the energy gap of the reset qubit. Usually the reset and computation qubits should be of different species as the reset qubits have a shorter relaxation time. The cooling limit would improve if the energy gap of the reset qubit is much larger than the one for the computation qubits. For instance, if an electron is used as the reset qubit and hydrogen nuclear spins for computation, this ratio would be $\frac{1}{660}$ which lowers the cooling limit by a factor of 660.

Figure 4 shows how the effective temperature decreases with increasing the number of computation qubits, $n$. It also shows that changing the $\frac{\Delta}{\delta}$ changes the cooling limit.

We can also answer one of the important questions about HBAC, namely, identifying how the performance of HBAC depends on the energy spectrum of the reset qubit.

The gap between the upper bound and the actual value gets looser as $\epsilon$, the polarization of the reset qubit increases.

Equation (2) can be generalized for arbitrary reset state, $\rho_R$. For a $D$-level reset system we get a similar condition as in equation (4) with the difference that the gap is replaced by the sum of the gaps. We refer to this as the “large gap” and use $\Delta$ to show it. The cooling limit depends linearly on the large gap.

It is interesting that despite the more complicated energy structure of the reset qubit, the “large gap” is the only parameter that would influence the cooling limit. In particular, the cooling limit does not directly depend on the number of energy levels or the spacing between them, as long as the total gap does not change.

This result also implies that a multi-qubit reset is linearly better than a single qubit reset. The energy gap of a multi-qubit reset system is the sum of the energy gaps of the individual qubits and as a result it has a larger gap which would improve the cooling limit. For instance, if $k$ identical qubits are used for the reset, then the energy gap would be $\Delta_{\text{total}} = k \Delta$ and it lowers the cooling limit by a factor of $\frac{1}{k}$.

Note that the energy structure of the reset system could still change the complexity or the number of operations for HBAC but the asymptotic state only depends on the largest gap of the reset system.

In conclusion, we find the fundamental limit of cooling for all HBAC techniques and show that it reduces exponentially with the number of qubits. It also depends on the ratio of the energy gap of the reset qubit to the gap of the computation qubits. We studied the effects of the changes to the energy spectrum of the reset system and showed that only the large gap of the reset system affects the asymptotic state. In particular, the number of energy levels, for a constant energy gap, does not influence the cooling limit.

Besides the fundamental significance, the cooling limit could have practical applications as well. For instance, it
could give a quantitative measure of imperfection for implementing and studying the HBAC. The natural choice would be the distance from the asymptotic state, \( \rho^\infty \), which requires the full density matrix. This may be expensive experimentally. The easier solution is \( |p_0 - p_0^\infty| \) which approaches zero as the state approaches to the asymptotic cooling limit.

For experimental implementation of HBAC, this measure quantifies how far the experiment is from the cooling limit and gives a metric for the assessment of the progress in the experiment.

Similarly, it can be used for theoretical cost analysis of HBAC which requires a notion of distance from the asymptotic state. The number of operations that are needed to achieve a certain fidelity to the asymptotic state, can be calculated in terms of \( |p_0 - p_0^\infty| \).

**Proofs and derivations.**

We restrict ourselves to diagonal density matrices for simplicity. It is shown in [12] that it is enough to study the diagonal density matrices for the purpose of HBAC.

The asymptotic state does not change under the operations of HBAC and is the fixed point of the dynamics. Technically this implies that if it is reset, it will still be sorted. The state after reset is \( \{ \rho^\infty = \{ p_0^\infty, p_1^\infty, \cdots, p_n^\infty \} \otimes \{ p_0 \} \} \), where the first part represents the state of the \( n \) computation qubits.

The fact that the full density matrix is sorted after the reset step, implies that \( p_i^\infty e^{-\epsilon} \geq p_{i+1}^\infty e^{\epsilon} \), \( \forall i \). On the other hand, the ratio of two consecutive diagonal elements of the density matrix never exceeds \( e^{2\epsilon} \) (see the supplementary information) which means that for the asymptotic state

\[
p_i^\infty e^{-\epsilon} = p_{i+1}^\infty e^{\epsilon}, \forall i.
\]

For a more detailed proof see the supplementary information.

Then the normalization of the state, \( \sum_i p_i^\infty = 1 = \sum_i e^{-2i\epsilon} p_0^\infty \) gives the:

\[
p_0^\infty = \frac{1}{\sum_i e^{-2i\epsilon}} = \frac{e^{-2\epsilon} - 1}{(e^{-2\epsilon})^{2n} - 1}.
\]

The reduced density matrix of the first qubit can be calculated by tracing other qubits and as we mentioned before, for a state \( \rho = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \), the polarization is

\[
P = \log \left( \frac{1}{\exp (-2(2^{n-1}) \epsilon)} \right) = 2^{n-1} \epsilon.
\]

The effective temperature of a qubit with the energy gap \( \delta \) is given by \( T_{\text{eff}} = \frac{\delta}{k_B \log \left( \frac{1}{\epsilon} \right)} \). For the first qubit it gives the equation [6].

For a \( D \)-level reset system with eigenenergies \( \{ E_1, E_2, \cdots, E_D \} \) which gives the reset state \( [\rho_R] = \begin{pmatrix} e^{-\frac{E_1}{K_B T}}, e^{-\frac{E_2}{K_B T}}, \cdots, e^{-\frac{E_D}{K_B T}} \end{pmatrix} \), again, we focus on the stopping condition which now changes to:

\[
p_i^\infty e^{-\frac{E_D}{K_B T}} \geq p_{i+1}^\infty e^{-\frac{E_1}{K_B T}}, \forall i.
\]

Similar to the qubit case, it can be shown that the distance between the consecutive probabilities is bounded by \( e^{-K_B T} \) (see the supplementary information) and therefore the equality holds.

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When the reset qubit is set, the ordering of the elements on the diagonal of the density matrix changes. These changes are what leads to the cooling eventually. The reset step takes the state \( \rho = \{\lambda_1, \lambda_2, \ldots, \lambda_{2^n+1}\} \) of \( n \) computation qubits and one reset qubit to

\[
\left[ \rho \right] = \left\{ p_0, p_1, \ldots, p_{2^n-1} \right\} \otimes \left[ \rho_R \right],
\]

where \( p_k = \lambda_{2^{i+1}} + \lambda_{2^i+2} \) and \( \left[ \rho_R \right] = \{a_1, a_2\} \). This can be generalized for the reset with a qudit \( \left[ \rho_R \right] = \{a_1, a_2, \ldots, a_k\} \) as well. Although the probabilities \( p_i \) are sorted, the full density matrix is not necessary sorted. For instance, for some indices \( i < j \), and \( m_i > m_j \), we could have

\[ p_i a_{m_i} < p_j a_{m_j}, \]  \hspace{1cm} (S1)

or similarly for some indices \( i > j \), and \( m_i < m_j \), we could get

\[ p_i a_{m_i} > p_j a_{m_j}. \]  \hspace{1cm} (S2)

In these cases, the sort operation in PPA would rearrange these (and probably other) terms and update the value of \( p_i \). We refer to the conditions in equation (S1) and equation (S2) as “crossing from below” and “crossing from above”.

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Supplemental Materials: The Asymptotic Cooling of Heat-Bath Algorithmic Cooling

PROOF OF THE ASYMPTOTIC STATE OF PPA AC

We first prove the convergence of the PPA algorithmic cooling. Once we know that the asymptotic state exist, we can easily use the argument in equation (2) to find the asymptotic state.

To prove the convergence, we first prove that \( p_0 \) converges and then the convergence of all the \( p_i \) follows from that. In order to make the connection between the convergence of \( p_0 \) and other \( p_i \), it is important to show that the distance between consecutive probabilities is bounded. This is proved in [1].

Before we get to the proof, it is useful to explain a few details about the dynamics and update rules of the PPA.

Crossings
respectively. The sort operator would swap \( p_i a_m \) with the appropriate term. For instance, when there is only one crossing from above, the updated \( p_i \) would be

\[
p_i' = p_i - p_i a_1 + p_{i-1} a_k. \tag{S3}
\]

Similarly for crossing from below we get

\[
p_i' = p_i - p_i a_k + p_{i+1} a_1. \tag{S4}
\]

For instance, consider \([\rho_R]=[...p_i,p_{i+1},...]*\{a_1,a_2\}\), where \(a_1+a_2=1\). If there is only one crossing between \(p_i\) and \(p_{i+1}\), namely \(p_{i+1}a_1 > p_i a_2\), then the sort operation rearranges the state to \([\rho_R]=[...p_i a_1,p_{i+1} a_1,p_i a_2,p_{i+1} a_2,...]\) which means that \(p_i' = (p_i + p_{i+1})a_1 = p_i - p_i a_2 + p_{i+1} a_1\).

In general, we can always write the updated \(p_i\) in a similar way.

The following two remarks that follow from the update rule, will also be useful.

**Remark 1.** Crossing from below increases the probabilities.

**Remark 2.** Crossing from above decreases the probabilities.

Both of these two remarks follows directly from the update rule in equation (S3) and equation (S4).

**Theorem 3.** Let \(p_i^0\) be the first diagonal element of the reduced density matrix of the computation qubits in the \(i^{th}\) iteration of PPA algorithmic cooling. Then \(\lim_{i \to \infty} p_i^0 = p_0^\infty\), for some constant \(p_0^\infty\).

**Proof.** The values \(p_i^0\) are increasing because it only can cross from below. It also is upper-bounded, therefore it must converge: \(p_0^\infty = \sup_i \{p_i^0\}\).

To prove the convergence for the rest of the \(p_i\) we need to first prove theorem (4) which requires the following definition. Consider two consecutive elements of the density matrix, \(p_i\) and \(p_{i+1}\). We define the following distance between the elements of the density matrix

\[
d_i \overset{\text{Def}}{=} \log \frac{p_i}{p_{i+1}}. \tag{S5}
\]

**Theorem 4.** For PPA algorithmic cooling with a reset qudit \([\rho_R]=[a_1,a_2,...,a_k]\) where \(a_j\) are sorted decreasing and sum to 1 and for any iteration \(j\), \(d_i^j \leq \log \frac{a_i}{a_k}\).

**Proof.** For our proof, we focus on the change of the distance \(d_i^j\) in some arbitrary iteration \(j\) and for some arbitrary \(i\) and show that it is upper bounded. Then we use the upper bound to prove the theorem.

For simplicity, we drop the superscript \(j\) and refer to the probabilities before the sort operation as \(p_i\) and after that with \(p_i'\). Similarly for the distance, \(d_i^j = d_i^{j+1}\) and \(d_i = d_i^i\).

The distance \(d_i\) could change in many different ways in an iteration of PPA (to become \(d_i'\)) but note that the change in \(d_i\) only depends on the changes of \(p_i\) and \(p_{i+1}\). This simplifies the analysis of the change in \(d_i\). There are few basic cases that \(p_i\) and \(p_{i+1}\) are affected and complicated situations could be analysed in terms of these basic cases. These cases are as follows:

- No crossing for either \(p_i\) or \(p_{i+1}\): \(d_i = d_i'\)
- Crossing between \(p_i\) and \(p_{i+1}\)
- Crossing between \(p_{j<i}\) and \(p_i\)
- Crossing between \(p_{j<i}\) and both \(p_i\) and \(p_{i+1}\).

The last two cases could also happen from below, \(j > i + 1\), and the proof is exactly the same for them.

We now show that in none of these case, the distance \(d_i^j\) can exceed the maximum of \(d_i\) and \(\log \frac{a_i}{a_k}\).

For the first case, the distance does not change.

For the second case, when there are \(t\) crossings between \(p_i\) and \(p_{i+1}\), the probabilities change to:

\[
p_i' = p_i + c
\]
\[
p_{i+1} = p_{i+1} - c,
\]
where \( c = f(t)p_{i+1} - (1 - f(k - t))p_i \) with \( f(t) = a_1 + a_2 + \ldots + a_t \). The proof is as follows:

\[
\frac{p'_i}{p'_{i+1}} = \frac{p_i + (p_{i+1} - p'_i)}{p'_{i+1}} = \frac{p_i + p_{i+1} - 1}{p'_{i+1}} - 1. \quad (S6)
\]

To find the upper bound we need a lower-bound for \( p'_{i+1} \).

\[
p'_{i+1} = (1 - f(k - t))(p_i + p_{i+1}) + (f(k - t) - f(t)p_{i+1} \geq (1 - f(k - t))(p_i + p_{i+1}) \geq a_k(p_i + p_{i+1}).
\]

This leads to

\[
\frac{p'_i}{p'_{i+1}} = \frac{p_i + p_{i+1}}{p_{i+1}} - 1 \leq \frac{1}{a_k} - 1 = 1 - \frac{a_k}{a_k} = \frac{a_1}{a_k}. \quad (S7)
\]

Next is to consider crossings between \( p_i \) and \( p_j, i < j \). In this case, \( p'_i \leq p_i \) and \( p'_{i+1} = p_{i+1} \) and as a result the distance \( d'_i \leq d_i \).

The last case is when \( p_{j<i} \) crosses both \( p_i \) and \( p_{i+1} \). In this case, both \( p_i \) and \( p_{i+1} \) are crossing from above and are decreasing. We need to show that their distance is still bounded by our upper bound.

We start by the simple case where there is only one crossing between \( p_{i+1} \) and \( p_j \), namely \( a_1 \geq p_j a_l \). In this case we have

\[
p'_i = p_i + c
\]

\[
p'_{i+1} = p_{i+1} - c,
\]

where \( c = p_{i+1} a_1 - p_i a_1 \) and \( c_2 = p_{i+1} a_1 - p_j a_j \). Note that \( c_1 \leq c \) and \( c_2 \leq c \). This implies that

\[
p'_i \leq p_i + c
\]

\[
p'_{i+1} \geq p_{i+1} - c.
\]

Therefore

\[
\frac{p'_i}{p'_{i+1}} \leq \frac{p_i + c}{p_{i+1} - c}.
\]

But we have already showed that \( \frac{p_i + c}{p_{i+1} - c} \leq \frac{a_1}{a_k} \).

The case that there are crossings can be similarly upper bounded.

So in all the possible cases, we get \( d'_i \leq \max \{ d_i, \log \left( \frac{a_1}{a_k} \right) \} \). Considering that \( d'_i = 0 \), initially all the distances were zero, for any iteration \( j \) and any index \( i \), we get

\[
d'_i \leq \log \left( \frac{a_1}{a_k} \right). \quad (S8)
\]

Now we use this to prove that all of the \( p_i \) converge.

**Theorem 5.** Let \( p'_i \) be the \( j^{th} \) diagonal element of the reduced density matrix of the computation qubits in the \( i^{th} \) iteration of PPA algorithmic cooling with a qubit reset \( |p_R\rangle = \frac{1}{e^{-2\epsilon} + e^{-\epsilon}} \{ e^\epsilon, e^{-\epsilon} \} \). Then the limit \( \lim_{i \to \infty} p'_i = e^{-2\epsilon} p_0^\infty \) exists. We refer to the limit as \( p_1^\infty \).

**Proof.** We already proved that the \( p_0^\infty \) exists. This means that

\[
\lim_{j \to \infty} (p_{j+1}^0 - p_0^0) = 0. \quad (S9)
\]

On the other hand, as \( j \to \infty \)

\[
p_{j}^{j+1} - p_0^j \to p_1^e \frac{e^\epsilon}{z} - p_0^j \frac{e^\epsilon}{z}. \quad (S10)
\]

The limit of the last term, \( p_0^j \frac{e^\epsilon}{z} \) exists and the left hand side converges as well, so \( \lim_{j \to \infty} p'_j \) should be \( e^{-2\epsilon} p_0^\infty \). The convergence of the rest of the \( p'_j \) follows by induction.

For the PPA with a reset qudit \( |p_R\rangle = \{ a_1, a_2, \ldots, a_k \} \), the proof is similar. As \( j \to \infty \) we get \( p_{j+1}^0 - p_0^j \to p_1^j a_1 - p_0^j a_k \) and as for the limit of \( j \to \infty \) the left hand side and the last term converge, so should the \( p_j \). The rest of the proof follows similarly.