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

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Introduction.—Purification of quantum states is essential for 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 quantum computation modalities, especially the ones that rely 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, at the expense of increasing the entropy of others [2,3]. An explicit way to implement this idea in ensemble quantum computers 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 cooling algorithms have been designed [6–11]. HBAC is not only of theoretical interest, experiments have already demonstrated an improvement in polarization using this protocol with a few qubits [12–18], where a few rounds of HBAC were reached, and some studies have even included the impact of noise [19].

Through numerical simulations, Moussa [7] and Schulman *et al.* [8] observed that if the polarization of the bath (ϵ_b) is much smaller than 2^{-n}, where n is the number of qubits used, the asymptotic polarization reached will be $\sim 2^{n-2}\epsilon_b$, but when ϵ_b is greater than 2^{-n}, a polarization of order one can be reached. Inspired also by the work of Patange [20], 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 general spin l, and extra qubits which get contact with a bath. We found the asymptotic limit by solving the evolution equation with the results supported by numerical simulation [7]. A proof has been reported by Raeisi and Mosca [21].

In this Letter we give the analytic result for the asymptotic polarization that can be reached when the initial state of the quantum computer is in the totally mixed state. This gives an achievable bound as we can always efficiently turn a state into the maximally mixed one, while some other initial states do lead to higher polarizations. We recover the limit of low polarization observed by Moussa and Schulman *et al.* We also show how a polarization of order one can be reached as a function of the number of qubits. We compare the 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 and cooling needed to get certain polarization.

HBAC 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 (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. 1).

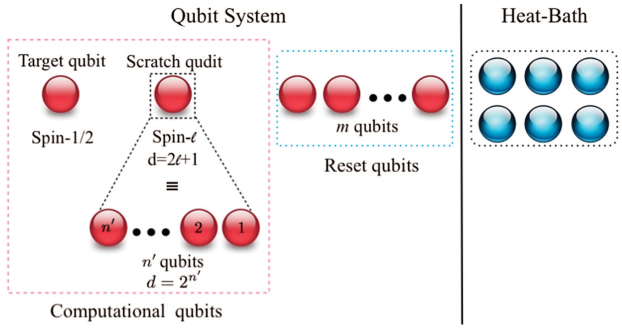

FIG. 1. HBAC can cool the target qubit by compressing entropy into m reset qubits and a d-dimensional spin l (or a string of qubits of Hilbert space of dimension d); then, HBAC pumps entropy from the qubit system into a heat bath by refreshing the m reset qubits.

The idea of HBAC is to first redistribute 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 by extracting entropy of the computational qubits. This process results in the cooling of the computational qubits while warming the reset qubits. The second step is to refresh the system using the heat bath for removing entropy.

For our study, we used a HBAC algorithm called the partner pairing algorithm (PPA), which was invented by Schulman *et al.* [8]. This protocol gives the optimal physical cooling of HBAC, in terms of entropy extraction, under the assumption that the refresh step rethermalizes the reset qubits with the heat bath [8,10]. In the PPA, the entropy compression operation U makes a descending sort of the diagonal elements of the system's density matrix. 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. 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.

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

$$\rho \overset{\text{compression}}{\rightarrow} \rho' = U\rho U^\dagger, \tag{1}$$

$$\rho' \overset{\text{refresh}}{\rightarrow} \rho'' = \mathrm{Tr}_{m_{\text{qubits}}}(\rho') \otimes \rho_{\epsilon_b}^{\otimes m}, \tag{2}$$

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.* [10], use $\epsilon = \mathrm{arctanh}\epsilon_b$ as polarization).

An interesting question is 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 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:

$$\rho = \rho''. \tag{3}$$

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

$$\mathrm{diag}(\rho_{\text{com}}) = (A_1, A_2, A_3, \ldots, A_{2d}), \tag{4}$$

where $\mathrm{diag}(\rho)$ is the vector of the diagonal elements of ρ. From this and Eq. (2), the state of the qubit system after a HBAC iteration will be described by

$$\mathrm{diag}(\rho'') = (A_1, A_2, \ldots, A_{2d}) \otimes \frac{1}{2^m}(1+\epsilon, 1-\epsilon)^{\otimes m}. \tag{5}$$

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. This will happen when we have the condition

$$A_i(1-\epsilon_b)^m \geq A_{i+1}(1+\epsilon_b)^m, \tag{6}$$

for $i = 1, 2, 3, \ldots, 2d-1$ (see Supplemental Material [22] for 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 (3).

Maximally mixed initial state.—If we start with a maximally mixed state, it is possible to show that (see Supplemental Material [22], a proof can be found in [21])

$$A_i^t(1-\epsilon_b)^m \leq A_{i+1}^t(1+\epsilon_b)^m, \tag{7}$$

where t labels the number of HBAC iterations. This is true for the initial step, as $A_i = (2d)^{-1}$ 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 Eqs. (6) and (7) indicates that the asymptotic state of the computational qubits can only go towards the equality

$$A_i^\infty(1-\epsilon_b)^m = A_{i+1}^\infty(1+\epsilon_b)^m, \tag{8}$$

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

From (8) and the property $\mathrm{Tr}(\rho_{\mathrm{com}}) = 1$, it is possible to find $A_i^\infty = [(1-Q)/(1-Q^{2d})]Q^{i-1}$, where $Q = [(1-\epsilon_b)/(1+\epsilon_b)]^m$. This result gives the exact solution of the steady state of the computational qubits $\tilde{\rho}_{\mathrm{com}}$ for all values of the bath polarization:

$$\mathrm{diag}(\tilde{\rho}_{\mathrm{com}}) = A_1^\infty(1, Q, Q^2, \ldots, Q^{2d-1}). \tag{9}$$

See Supplemental Material [22] for details.

Asymptotic polarization.—From the steady state [Eq. (9)], the asymptotic polarization of the target qubit is

$$\epsilon_{\mathbb{1}}^\infty = \frac{(1+\epsilon_b)^{md} - (1-\epsilon_b)^{md}}{(1+\epsilon_b)^{md} + (1-\epsilon_b)^{md}}. \tag{10}$$

The corresponding temperature of the target qubit will be $T_{\mathrm{steady}} = (1/md)T_b(\Delta E_t/\Delta E_r)$ ($d = 2^{n'}$ 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 [23,24].

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

In the limit for low bath polarization, $\epsilon_b \ll 1/md$, 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. 2, as a function of the bath polarization for a different number of qubits, using Eq. (10). We can observe the transition noted by [7] and [8] 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 (10). Then,

$$\Delta_{\max} = \frac{2}{e^{md\ln[(1+\epsilon_b)/(1-\epsilon_b)]} + 1} = \frac{2}{e^{m2^{n'}\ln[(1+\epsilon_b)/(1-\epsilon_b)]} + 1}. \tag{11}$$

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. 2, we show $\epsilon_{\mathbb{1}}^\infty$ as a function of ϵ_b for different values of d, with $m = 1$.

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. (7).

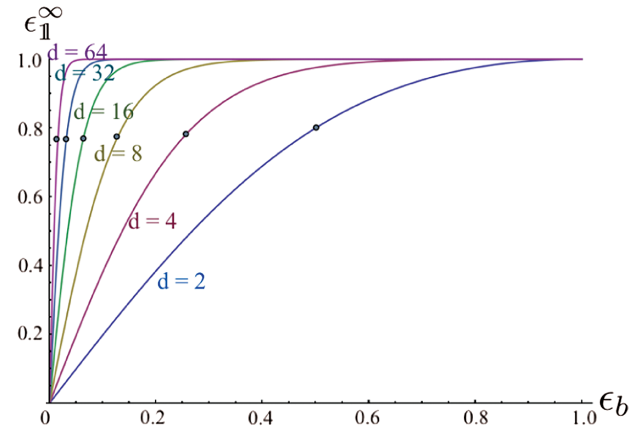

FIG. 2. Asymptotic achievable polarization for the target qubit. This polarization increases double exponentially in the number of qubits as the scratch qudit n'. The dots are located at the point of $\epsilon_{\mathbb{1}}^\infty$ which corresponds to the $\epsilon_b = 1/md$, where the transition can 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.)

Numerical simulation indicates that this could also happen with some initial states not obeying Eq. (7). But we can also find explicit examples of initial states that lead to asymptotic polarizations that are higher than Eq. (10). As any state can be efficiently maximally randomized, it is always possible to reach the polarization given Eq. (10) and maybe do better if the initial state is different.

Schulman's physical-limit theorem.—The steady state, Eq. (9), is consistent with the 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 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

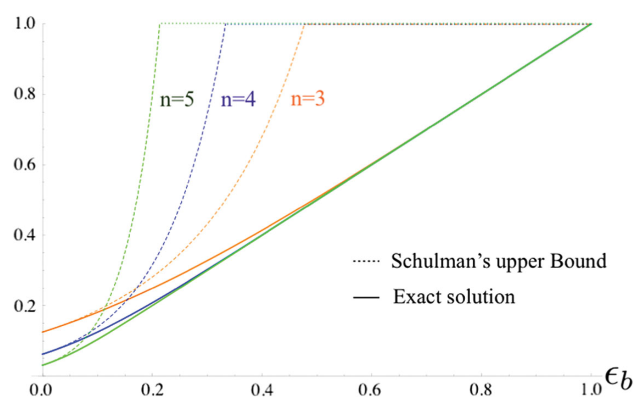

FIG. 3. Upper limit of the probability of any basis state for the total n qubit system ($n = n' + 2$: $n' + 1$ computational qubits and one reset qubit). The dashed line corresponds to the Schulman's upper bound and the thick line to the exact asymptotic probability. Orange represents $n = 3$, blue represents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

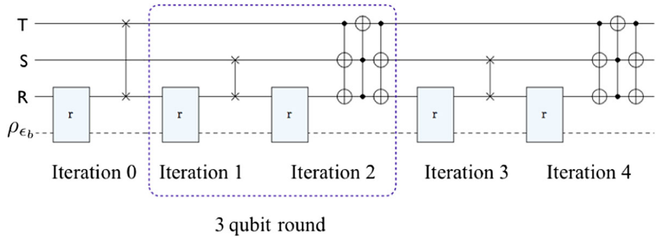

FIG. 4. Quantum circuit for the PPA method on a system of 3 qubits starting in the total mixed state. In the circuit diagram, the target, the scratch, and the reset qubits are denoted T, S, and R, respectively; the dashed line corresponds to the heat bath and r stands for the refresh operation. The figure 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 3 qubit round).

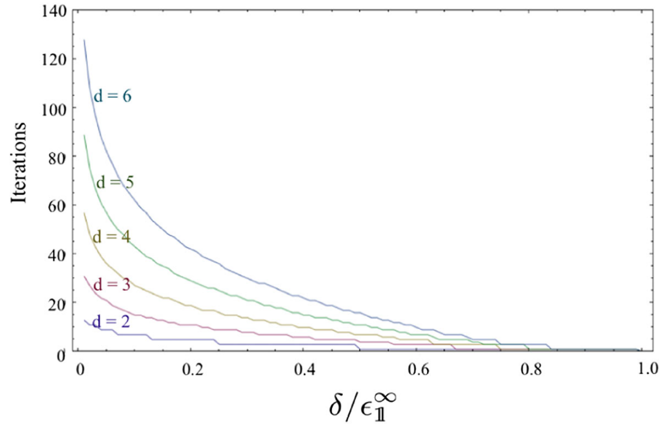

FIG. 5. The PPA steps required to have polarization $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$ as a function of $\delta/\epsilon_{\mathbb{1}}^{\infty}$, for $d = 2$, 3, 4, 5, and 6.

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 $|00\ldots0\rangle$ at the cooling limit: $p_{\max} = A_1(1+\epsilon_b)/2$ [from Eq. (9) and $\rho = \tilde{\rho}_{\rm com} \otimes \rho_{\epsilon_b}$]. That expression can be written as a function of n and ϵ_b as follows $p_{\max} = \epsilon_b/\{1 - [(1-\epsilon_b)/(1+\epsilon_b)]^{2^{n-1}}\}$.

Figure 3 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 differs for large values of ϵ_b.

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 3 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. 4.

Consider that the polarization of the first qubit is ϵ^t after the tth iteration. Applying two more iterations, which corresponds to the 3 qubit round in Fig. 4, the polarization of the target qubit increases from ϵ^t to ϵ^{t+2} as follows:

$$\epsilon^{t+2} = 2ab\epsilon^t + \epsilon_b, \tag{12}$$

where $a = [(1+\epsilon_b)/2]$ and $b = [(1-\epsilon_b)/2]$.

Let t start from 0, then $\epsilon^0 = \epsilon_b$ after the first iteration. From Eq. (12), the polarization after applying j 3 qubit rounds can be written as

$$\epsilon^{t=2j} = \epsilon_{\mathbb{1}}^{\infty} - q^j(\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b), \tag{13}$$

where $q = [(1-\epsilon_b^2)/2]$. Using (10) with $d = 2$, we have that the corresponding asymptotic polarization $\epsilon_{\mathbb{1}}^{\infty} = [2\epsilon_b/(1+\epsilon_b^2)]$. From this equation we can find the number of steps needed to get to $\epsilon = \epsilon_{\mathbb{1}}^{\infty} - \delta$,

$$N(\delta, \epsilon_b) = 2j = 2\frac{\log[\delta/(\epsilon_{\mathbb{1}}^{\infty} - \epsilon_b)]}{\log q}. \tag{14}$$

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

$$N_{\text{upper bound}} = \prod_{k=1}^{k=[n'/2]} N(\delta_k, \epsilon_k), \tag{15}$$

where $\epsilon_{\max} = \{[(1+\epsilon_b)^{d/2} - (1-\epsilon_b)^{d/2}]/[(1+\epsilon_b)^{d/2} + (1-\epsilon_b)^{d/2}]\}$; $\epsilon_k := f(\epsilon_{k-1}) - \delta_k$; $\epsilon_{h,\delta} = \epsilon_h$, with $h = [n'/2]$ (the integer part of $n'/2$); $f(\epsilon) = [2\epsilon/(1+\epsilon^2)]$; $N(\delta,\epsilon) = 2(\log\{\delta/[f(\epsilon_b) - \epsilon_b]\}/\log q)$; and $\epsilon_0 = \epsilon_b$. (More details are in the Supplemental Material [22].)

Figure 5 shows numerical simulations of the number of steps as a function of $\delta_{\rm rel} = [(\epsilon_{\mathbb{1}}^{\infty} - \epsilon)/\epsilon_{\mathbb{1}}^{\infty}] = \delta/\epsilon_{\mathbb{1}}^{\infty}$. The simulations are consistent with the upper bound of the number of steps and with the exact solution for the case of 3 qubits.

Conclusion.—HBAC is a process to purify a number of qubits by removing entropy 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 ϵ_b. From this formula we can understand the transition of behavior of the asymptotic polarization at $1/md$. 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. 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 asymptotically reached. If conditions (7) are not obeyed, it may be possible to reach higher polarization. Finally, we obtained the number of steps required to reach a given polarization for a specific number of qubits [25].

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