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No-go theorem for ground state cooling given initial system-thermal bath factorization

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Ground-state cooling and pure state preparation of a small object that is embedded in a thermal environment is an important challenge and a highly desirable quantum technology. This paper proves, with two different methods, that a fundamental constraint on the cooling dynamic implies that it is impossible to cool, via a unitary system-bath quantum evolution, a system that is embedded in a thermal environment down to its ground state, if the initial state is a factorized product of system and bath states. The latter is a crucial but artificial assumption included in numerous tools that treat system-bath dynamics, such as master equation approaches and Kraus operator based methods. Adopting these approaches to address ground state and even approximate ground state cooling dynamics should therefore be done with caution, considering the fundamental theorem exposed in this work.

In the quantum regime, ground-state cooling of a small object that is embedded in a thermal environment, such as neutral atoms[1], ion traps[2], mechanical resonators[3,4], nuclear spins (polarization)[5], is an intriguing challenge and one of the most desirable of quantum technologies[6]. Mathematically, a ground-state cooling (or polarization) process can be formulated as a transformation from the initial state of the system + bath to a final state, where the small object, the "system", reaches its ground state. There have been variety of ground state cooling schemes, for example, sideband cooling[1], which have been carried out experimentally[7–9]. Here we prove that a fundamental constraint on the cooling dynamic implies that it is impossible to cool, via a unitary system-bath quantum evolution, a system that is embedded in a thermal environment down to its ground state, if the initial state is a factorized product of system and bath states. The latter is a crucial but an artificial assumption often included in many descriptions of system-bath dynamics[10]. This no-go theorem more generally implies that, with a factorized system-thermal bath preparation, quantum evolution cannot drive a system to a pure state. We prove this no-go theorem by using the properties of unitary transformations. We also provide counter examples that can result in ground state cooling: the cases when the environment is prepared in a non-thermal state, and a scenario with the system-bath being initially correlated.

Note that this theorem addresses "ground state cooling", i.e. an ideal cooling to the exact system ground state. As such, the goal is the ideal limiting case of many experiments in which the target is cooling to near the ground state. The result provides a formal proof with significant consequences for theoretical and computational studies[11–14].

Results

Unitary constraint of system + bath. To prove this fundamental statement we consider a generic arrangement with a small entity, comprising a few degrees of freedom, referred to as the "system" possibly subjected to time dependent fields, interacting with a bath that is in a thermal equilibrium state. The total Hamiltonian is given by

$$H = H_S + H_B + H_{SB}, \qquad (1)$$

where H_S is the Hamiltonian of the system, H_B is that of the thermal bath, and H_{SB} denotes the system-bath interaction Hamiltonian. The details of these terms, whether controllable or uncontrollable (time-dependent or not), do not alter our results. Time evolution in quantum mechanics is dictated by a propagator $U(t_f, t_0)$, which transfers the full initial system + bath density matrix $\rho(t_0)$ to the final density matrix $\rho(t_f)$,

$$\rho(t_f) = U(t_f, t_0)\rho(t_0)U^\dagger(t_f, t_0) \qquad (2)$$

Since H is Hermitian, the unitary condition $U(t_0, t_f)U^\dagger(t_0, t_f) = U^\dagger(t_f, t_0)U(t_f, t_0) = I$ is satisfied, I is the unity operator, and the trace of the density matrix ρ is preserved. Without loss of generality, the initial state of the total system is assumed here to be diagonal, $\rho(t_0) = \mathrm{diag}(P_0, P_1, \ldots)$. If it is non-diagonal, we can diagonalize it by a unitary operator W such that $\mathrm{diag}(P_0, P_1, \ldots) = W\rho_0 W^\dagger$. The set $\{P\}$ corresponds to the eigenvalues of $\rho(t_0)$, and we order the eigenvalues according to their magnitude, $1 > P_0 \geq P_1 \geq \ldots$. Similarly, without loss of generality, we can also assume a diagonal form for the final state, $\rho(t_f) = \mathrm{diag}(Q_0, Q_1, \ldots)$, again ordered as $1 \geq Q_0 \geq Q_1 \geq \ldots$. The set $\{Q\}$ corresponds to the eigenspectra of $\rho(t_f)$. If $\rho(t_f)$ is not diagonal, it can be diagonalized with a unitary matrix, $\mathrm{diag}(Q_0, Q_1, \ldots) = V^\dagger\rho(t_f)V$. Overall, we can redefine the time evolution operator U as VUW, a unitary operator, to ensure that both initial state and final state are diagonal matrices. The density matrices $\rho(t_f)$ and $\rho(t_0)$, Hermitian operators, are connected by a unitary (rotation) operation, thus they must have identical eigenspectra, i.e., $\{Q\} = \{P\}$. Since the elements are ordered, we can relate them one by one,

$$P_k = Q_k, \quad k = 0, 1, 2\ldots \qquad (3)$$

We now define d_0 and d_f as the number of non-zero eigenvalues in the set $\{P\}$ and $\{Q\}$, respectively. Under a unitary evolution, d_0 must be equal to d_f, a prerequisite for relation (3) to hold (or $d_0/d_f = 1$ when d_0 goes to infinity).

No-go theorem. Based on these simple considerations, we argue next that under system-bath unitary operations, acting on system or bath or both, one *cannot* cool a mixed system state down to its ground state if the total density matrix is initially system-bath factorizable and the bath is thermal. That is, the process

$$\rho(t_0) = s \otimes b \rightarrow |0\rangle\langle 0| \otimes B = \rho(t_f) \qquad (4)$$

cannot be carried out with a unitary matrix U (even if it operates on both the system and bath). The left hand side in Eq. (4) describes the initial system-bath product state. Here, $s = \mathrm{diag}(s_0, s_1, \ldots)$ denotes the system density matrix at t_0, which is anything but a pure state, and $b = \mathrm{diag}(b_0, b_1, \ldots)$ denotes the bath state at that time, a thermal state at nonzero temperature. The right hand side of Eq. (4) includes the target final state where the system has been cooled down to its ground state $|0\rangle$ and the bath is a mixed state $B = \mathrm{diag}(B_0, B_1, \ldots)$ which is a diagonal matrix[11–13]. We now provide an argument, which shows that one cannot evolve between these initial and final states via unitary dynamics.

Define N_S and N_B as the Hilbert space dimension of the system and bath, respectively. If the bath is initially thermal and s is not a pure state, the inequality $d_0 > N_B$ holds. In particular, if the system is initially thermalized we reach the upper bound $d_0 = N_S N_B$. On the other hand, the target state $\rho(t_f)$ has only $d_f \leq N_B$ nonzero eigenvalues, reaching the bound $d_f = N_B$ if the bath becomes a thermal state at time t_f. Since $d_f < d_0$, equation (3), written here in the form

$$s_m b_j = B_k \qquad (5)$$

cannot be satisfied. Here the index m counts the system eigenvalues, j and k follow the bath eigenvalues. Hence, system-bath unitary operations cannot cool a system coupled to a thermal bath down to its ground state if the system-bath initial state is factorizable and the system is initially in a mixed state. The analogous proof holds for any final pure state of the system. While previous studies have pointed out the unattainability of the absolute zero of in such situations[15–17], here we isolate the centrality of the factorization assumption, and emphasize its strong implications regarding both the underlying

physics and the suitability of master-equation type computational frameworks that often assume factorization, see e.g., Ref. 11–14.

Related cases. It is of interest to examine a few related situations. First, if the system is prepared in a pure state, we find that $d_0 = N_B$, and ground state cooling can potentially be performed if Eq. (5) is satisfied. Second, one can achieve ground state cooling by preparing the bath in a non-thermal state. In this case we consider an initial bath state b with N'_B nonzero eigenvalues, $N'_B < N_B$. This results in $d_0 > N'_B$ while $d_f \leq N_B$. These values could be made identical if the states b and B are very different. As the simplest example, consider both the system and the "bath" as single qubits, where initially the "bath" populates its ground state, $b_0 = 1$. Using Eq. (5), matching eigenvalues, we require that $s_0 = B_0$. The system ground state can therefore be reached here by the swapping operation. A more involved scenario includes a two-qubit bath and a single-qubit system where we initially set the system in a mixed state while we prepare the bath in a non-thermal state with precisely two zero eigenvalues, $b_2 = 0$ and $b_3 = 0$. The prerequisite for ground state cooling, $d_0 = d_f$, could be fulfilled here if at the end of the quantum evolution all four bath eigenvalues $B'_i s$ are made nonzero, resulting in $d_0 = d_f = 4$.

Third, we note that system-bath *correlated* initial states[18] do allow for ground state cooling. We illustrate this possibility by modeling the system as a qubit, with ground state $|0\rangle$ and excited state $|1\rangle$. We construct the following correlated initial state

$$\rho(t_0) = |0\rangle\langle 0| \otimes b^{(0)} + |1\rangle\langle 1| \otimes b^{(1)} \qquad (6)$$

where $b^{(0)} = \mathrm{diag}(b_0, \ldots, b_n)$ and $b^{(1)} = \mathrm{diag}(b_{n+1}, \ldots, b_{N_B})$. As before, the target state is $\rho(t_f) = |0\rangle\langle 0| \otimes B$. It is easy to confirm that the prerequisite for ground state cooling is satisfied, and the number of non-zero eigenvalues for the initial and final density matrices is identical, $d_0 = d_f = N_B$. Furthermore, one could pair the eigenvalues one by one, as required by Eq. (3). For example, we can set the system with $s_0 = s_1 = \frac{1}{2}$ and the bath with $\frac{b_k}{2} = B_k$. As a result, the reduced density matrix of the bath is the same, initially and finally, whereas the reduced density matrix of the system at time t_0 is $(|0\rangle\langle 0| + |1\rangle\langle 1|)/2$, for a given n such that $b_0 + \ldots + b_n = 1/2$.

Approximate cooling and an alternative proof. We now consider *approximate* ground state cooling, defined as the evolution from the initial state $\rho(t_0) = s \otimes b$ to the final-factorizable state $\rho(t_f) = S \otimes B$, where $S = \mathrm{diag}(S_0, S_1, \ldots)$, the diagonal state of the system at the final time, describes a system "colder" than the initial one, in the sense that S has fewer nonzero elements than s. This situation is typically assumed in the framework of Markovian master equations[19]. Since the underlying quantum dynamics is unitary, we should be able to match the eigenvalues of the initial state and the final state. In particular, the first two eigenvalues should fulfill $s_0 b_0 = S_0 B_0$ and $s_0 b_1 = S_0 B_1$. The second relation holds in the case where the system energy gap, between its ground state and first excited state, is larger than the corresponding gap in the bath, $s_0 b_1 > s_1 b_0$. These relations yield $B_1/B_0 = b_1/b_0$, translated to $e^{-(E_1-E_0)/K_B T_i} = e^{-(E_1-E_0)/K_B T_f}$ (K_B is Boltzmann constant), if we further demand that the bath internal spectra is identical at t_0 and t_f, and that the bath acquires a thermal equilibrium state at the final time[10,11,12]. Here T_i and T_f denote the temperature at the different times. The last relation implies that the final-time temperature is equal to the initial-time temperature, i.e., the bath has not been changed through the cooling process, $\{b\} = \{B\}$. As a result, to satisfy Eq. (3), we must conclude that the system retains all its values, $S_m = s_m$. In the scenario described here, quantum evolution *cannot* modify the *system* population. Thus, even an approximate ground state cooling is impossible, as long as the system ground state is nondegenerate. Note that this argument provides a supportive proof for the impossibility of ground state cooling if we take $S_0 = 1$ and $S_{m \neq 0} = 0$.

Discussion

Ground state cooling within system-bath unitary operations is not possible given initial system-thermal bath factorization. The linearity of unitary operations has, in the past, resulted in a no-go theorem, the no-cloning theorem[20], one of the building blocks in modern quantum information theory. Our no-go principle is similarly based on unitary evolution, and stands at the foundation of any theory that aims at describing ground state cooling and pure state preparation. For example, many recognized master equation techniques, as well as Kraus operator based methods[10], are predicated on the initial factorization of the system and bath. Adopting these approaches to address issues of cooling should be done with caution, considering the fundamental constraint exposed in this work.

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Author contributions

L.W. performed the initial proof of the presented no-go theorem. L.W., D.S. and P.B. discussed the results and implications at all stages, and wrote the manuscript.

Additional information

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