Absolute Dynamical Limit to Cooling Weakly Coupled Quantum Systems

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Here we address the question of just how cold one can cool a quantum system, given that the size of the control forces is limited. We solve this problem fully, within the dual regimes of (i) weak coupling, defined as that in which the thermalization dynamics of the system is preserved, and (ii) relatively strong control, being that in which appreciable cooling can be achieved. State-of-the art cooling schemes are presently implemented in this regime. Given that the maximum rate of coupling to the system is bounded, we identify a control protocol for cooling, and provide detailed structural arguments, supported by strong numerical evidence, that this protocol is globally optimal. From this we obtain simple expressions for the absolute limit to cooling. The methods developed can also be used to obtain optimal controls for a broad class of state-preparation problems.

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Preparing quantum systems in pure states is important for potential quantum technologies [1–4]. This task is strongly linked to ground-state cooling, as both require that all the entropy is extracted from the system. As such, there is a great deal of interest in cooling mechanical resonators, and a number of cooling schemes of increasing effectiveness have been proposed [5–9]. Since the forces used to implement cooling are always limited, the question of what ground-state population can be achieved for a given maximum control force is of both fundamental and practical importance. There are two distinct regimes of cooling: either the dynamics of the thermal relaxation is preserved under the control (weak coupling to the controller) or it is not (strong coupling). Here we consider optimal cooling in the former. Within this regime, our analysis is also applicable to the preparation of arbitrary pure states under general Markovian noise processes.

The complexity of cooling and state preparation is due to the interplay of coherent (unitary) and incoherent (irreversible) dynamics. Furthermore, it is usually impossible to prove the optimality of control protocols for dynamical systems in which the state space is unbounded and the controls constrained. Thus, to determine the fundamental limits to cooling by quantum control, we adopt a heuristic approach: we attempt to analyze the structure of the cooling problem in sufficient detail to make a well-justified guess as to the optimal protocol. We test the optimality of this protocol by comparison with those found using numerical optimization. We obtain very strong analytical and numerical evidence that our protocol is globally optimal and thus determines the absolute dynamical limit to cooling in the dual regimes of weak coupling and high fidelity control.

In this Letter, we consider the most general setting in which an N-dimensional "target" system can be cooled: the target system is coupled to a second, M-dimensional "auxiliary" system via an interaction Hamiltonian H_{I}, whose eigenvalues we denote by $\hbar\lambda_j$. This Hamiltonian, coupled with any trace-preserving operation on the auxiliary, implements the cooling process [10]. The constraint we impose on the speed of control is that $|\lambda_j| \leq g$, $\forall j$, for some rate constant g. For a given experimental scenario, one calculates the eigenvalues λ_j by (i) determining the full Hamiltonian H for the combined target and auxiliary systems, (ii) removing all contributions to H that are proportional to the identity when traced over either of the systems, and (iii) calculating the eigenvalues of the matrix that remains. While the limit we obtain applies to every-state preparation scheme, we note that other constraints may be more appropriate in different scenarios. Our constraint is appropriate for coherent coupling between target and auxiliary, and this is used by state-of-the-art experiments [2–4].

Here we focus on preparing the maximal ground-state population at a single time, rather than in the steady state. We do this because (i) the former is essential for quantum information processing and other tasks that require coherence with which cooling would interfere, and (ii) our analysis below suggests that the optimal ground-state population cannot be reached in the steady state.

To proceed we must choose a model of thermalization, and the Redfield master equation is the obvious choice [11]: it describes accurately any weakly damped Markovian quantum system, and weakly damped systems are the most important for quantum technologies. [The Redfield master equation equates to the usual quantum-optical master equations for the harmonic oscillator and two-level system (qubit) [11].] We assume that the energy levels of the system are not altered appreciably by the control interaction, meaning that the energy gaps are

much larger than g. This is the weak coupling regime and is what decouples the master equation for the target from the time-dependent control Hamiltonian. We also choose the auxiliary system to be ideal: it has large enough energy gaps to sit in its unique ground state at the ambient temperature T and is not subject to any damping or decoherence (we will show that damping the auxiliary does not improve cooling). Present cooling methods for ions and nanoresonators are essentially ideal in the first manner, but not the second. We note that an undamped auxiliary is only optimal for cooling because we ignore the practical issue of its reinitialization, but this is permissible because the damping of the auxiliary could be controlled by time-dependent coupling to a third system.

Since the control takes the target out of equilibrium, the bath induces an irreversible relaxation of the system *during* the cooling process, so we must understand how the control and damping act together. Fortunately, the regime in which cooling is most useful, and the primary goal of experiments, is that in which the target is cooled very close to the ground state. This requires that the damping (thermalization) rate of the system γ satisfies $\gamma(\bar{n}+1)/g \equiv \varepsilon \ll 1$ (where $\bar{n}$ is defined below), allowing us to perform an analysis to first order in ε. Defining $\mathcal{D}(c)\rho \equiv (c^\dagger c\rho + \rho c^\dagger c)/2 - c\rho c^\dagger$ for an operator c, the master equation that describes thermalization of a qubit is $\dot{\rho} = -\gamma[(1+\bar{n})\mathcal{D}(\sigma) + \bar{n}\mathcal{D}(\sigma^\dagger)]\rho$, where $\bar{n} = e^{-\hbar\omega/kT}/(1-e^{-\hbar\omega/kT})$. Here, $\hbar\omega$ is the energy gap, σ is the lowering operator, and the equilibrium population of the excited state is $P_T = \bar{n}/(1+2\bar{n})$. For a harmonic oscillator the master equation is the same, but with the replacement $\sigma \to a$, and ω and $\bar{n}$ become, respectively, the oscillator frequency and the thermal occupation number.

The full system to be studied is thus given by

$$\dot{\rho} = -(i/\hbar)[\mathcal{H}_{tg} + \mathcal{H}_I + \mathcal{H}_x, \rho] + \mathcal{L}\rho, \qquad (1)$$

where $\mathcal{H}_{tg}$ and $\mathcal{H}_x$ are, respectively, the target and auxiliary Hamiltonians, and $\mathcal{L}\rho$ represents the thermal terms given above. To achieve our goal we must determine the optimal choice of the auxiliary and interaction Hamiltonians $\mathcal{H}_x$ and $\mathcal{H}_I$ (subject to the constraint described above) and any trace-preserving operations on the auxiliary to maximize the target's ground-state population $P_g(t) = \mathrm{tr}(\rho|0\rangle\langle 0|_{tg} \otimes I_x)$ at some final time t. To arrive at our conjectured optimal cooling protocol, we examine the relationship between the structure of ρ, the role of $\mathcal{H}_x$ and trace preserving operations on the auxiliary, and the thermal dynamics of the target.

First we examine ρ. We denote the energy levels of the target by $|m\rangle$ and those of the auxiliary by $|j\rangle_x$. The target is initially in thermal equilibrium, and the auxiliary in its ground state $|0\rangle_x$. We depict the matrix elements of ρ in Fig. 1. Each subblock of this matrix is the full state space of the auxiliary and corresponds to a single state of the target. The initial populations appear in the elements labeled by A_j, and are thus in different subblocks. Thus, if we ignore the continual thermalization dynamics, the coldest target state is achieved by transferring all the population to the subblock in the upper left-hand corner. The essential observation we need is that cooling is a process of population transfer between orthogonal subspaces.

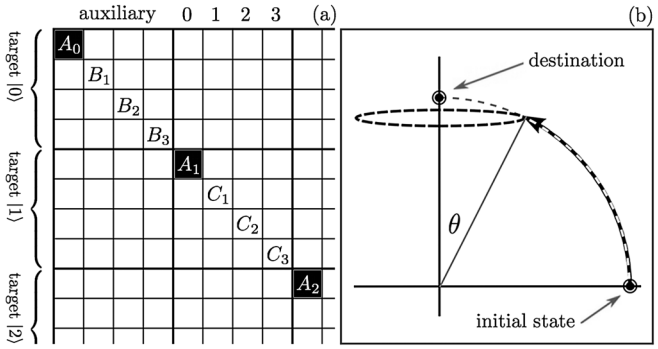

FIG. 1. (a) Depiction of the density matrix for the joint state of the target and auxiliary. The auxiliary states are the "fast" index, illustrated here with $M = 4$. (b) A schematic depiction of the geometry of quantum dynamics, showing why rotations in the local subblocks do not change the angle to go for the cooling rotation. This rotation is the dashed arrow, and the dashed ellipse is the motion of a local rotation.

For $\mathcal{H}_x$ and $\mathcal{H}_I$, we can use insights from the geometry of quantum dynamics [12]. The first of these is that, given the constraint above, the fastest way to take any initial pure state to any other state is via a geodesic, the equivalent of a great circle in real vector spaces. The rotation angle along this "great circle" is determined by the inner product between the current and final states. The minimum time to get from any state $|1\rangle$ to an orthogonal state $|2\rangle$ is $\tau = \pi/(2g)$, and is achieved by the Hamiltonian $H = g(|1\rangle\times\langle 2| + |2\rangle\langle 1|)$; this "quantum speed limit" can also be extended to mixed states [13]. This shows that in the absence of damping (thermalization), the fastest way to perform the cooling operation is to rotate each of the excited states A_j to the corresponding unpopulated states B_j $(j > 1)$ at the maximum rate.

Consider a cooling rotation taking an initial state $|A\rangle$ to an orthogonal state $|B\rangle$, so that $|\psi(t)\rangle = \cos\theta|A\rangle + \sin\theta|B\rangle$, where the angle $\theta = gt$. The local Hamiltonians $\mathcal{H}_{tg}$ and $\mathcal{H}_x$ cannot change θ. This can be seen by either (i) examining the matrix in Fig. 1 and applying the geometry of vector spaces or (ii) observing that $\mathcal{H}_{tg}$ and $\mathcal{H}_x$ preserve the entropy of either system, and changing θ changes these entropies. In addition, switching to the interaction picture shows that the effect of any local Hamiltonian can be obtained by allowing H_I to vary with time. Thus, in optimizing the time-dependent control protocol we can set the local Hamiltonians to zero.

Using the above observations we can now show the following.

Theorem: If (i) the target interacts only with the auxiliary (no heating) and (ii) the auxiliary has at least the dimension of the target ($M \geq N$), then no completely positive trace-preserving operation on the auxiliary can increase the maximum possible ground-state population of the target at any future time.

Proof: Since $M \geq N$, the auxiliary A can transfer the populations of all target basis states at the maximal rate. All completely positive trace-preserving operations on A can be obtained by performing a joint unitary U between A and a third system S. Now enlarge A to include S, meaning that the interaction also now includes S. Call the new auxiliary A', and the new interaction H_{I}'. Since U is local to A' it cannot change θ. And since H_{I} lies within a strict subset of H_{I}', it provides no advantage over the latter [14]. ■

We now consider the role of $\mathcal{L}$, the continual thermalization of the target during the control process. We first present an argument that gives strong support for the following simple and rather remarkable statement: all optimal cooling protocols will achieve the maximal ground-state population just prior to a time $\tau = \pi/(2g)$, and will do so only when the system starts in equilibrium. This argument is as follows. The thermal master equation gives transition rates between the diagonal elements of ρ and decay rates for all off-diagonal elements (in the energy basis). As soon as the ground-state population P_{g} rises above its equilibrium value, there is a net thermal transition rate out of the ground state to states orthogonal to it. The population taken out of the ground state can be returned by transferring it to the auxiliary, which, as established above, will require a minimum time τ. During this time, a further amount of population $P(\tau)$ will be taken out by thermalization. However, we will never be able to transfer this back to the ground state, as this population will again flow out by the time we have transferred it all back. Furthermore, since population transfer is a rotation on the unit sphere, the rate of the increase of P_{g} goes to zero as t approaches τ. Since the exit rate from the ground state is nonzero at $t = \tau$, no matter how large $g/(\bar{n}\gamma)$, there will always be a time slightly prior to τ at which we lose by waiting longer. Finally, since the outward transition rate increases as P_{g} moves away from equilibrium, $P(\tau)$ will only be minimal when P_{g} *starts* at its equilibrium value. This implies that the maximal cooling can only be obtained instantaneously; no steady-state cooling protocol can achieve this maximum.

To obtain our proposed optimal $\mathcal{H}_{\mathrm{I}}$, we need to examine *where* thermalization places the population that leaves the ground state. For qubits and harmonic oscillators, thermal transitions occur only between adjacent energy levels, and so we focus on this here (the analysis readily generalizes). To first order in $\gamma\bar{n}\tau = \pi\gamma\bar{n}/(2g) \ll 1$, population from A_0 goes to A_1, and from B_j to C_j, $\forall\, j$ (see Fig. 1). While the populations leaked to A_1 and C_j are small, to obtain optimal cooling to first order in ε we must optimally transfer these populations to the ground state. As A_1 is already rotated to B_1, and since the leakage is small and distributed over the transfer path, the leakage to A_1 is already handled optimally. The populations that appear in the C states can be rotated to additional states in the B subspace if these are available (if M is large enough). We can now conclude that (i) nothing can be done to retrieve the populations in the C states if $M \leq N$, and (ii) once the Hamiltonian is chosen to rotate all the C states to the ground state, all the first-order leakage is handled optimally.

If our protocol is indeed optimal, then given the structure of the thermal transition rates in harmonic oscillators and single qubits, the maximum cooling can be achieved with an auxiliary dimension $M = 2N - 1$ and the majority of the cooling with $M = N$. The optimal interaction Hamiltonian would be $\mathcal{H}_{\mathrm{I}}^{\mathrm{opt}} = G + G^{\dagger}$, where

$$G = g \sum_{j=1}^{\min(M,N)-1} |0, j\rangle\langle j, 0| + g \sum_{j=N}^{\min(M-1,2N-2)} |0, j\rangle\langle 1, j - N + 1|, \qquad (2)$$

and $|n, m\rangle = |n\rangle_{\mathrm{tg}} \otimes |m\rangle_{\mathrm{x}}$. This interaction is not linear, and shows that to achieve the best control under the constraint, *all* the eigenvalues of H_{I} must be maximal ($|\lambda_j| = g$, $\forall\, j$). For cooling resonators, in which the interaction is typically linear, it may be possible to get closer to $\mathcal{H}_{\mathrm{I}}^{\mathrm{opt}}$ by using multiple qubits as the auxiliary and introducing nonlinearities in the resonator degrees of freedom.

To verify the optimality of $\mathcal{H}_{\mathrm{I}}^{\mathrm{opt}}$ we turn to numerical optimization [16]. We perform a search over all Hamiltonians of the joint system, including piecewise-constant time dependence, under the constraint, for different cooling times and different auxiliary dimensions up to $M = 5$. The thermal dynamics of a target for $N > 2$ is somewhat arbitrary, since it depends on the energy gaps. Here we just use the master equation for an oscillator truncated at N [17]; the Boltzmann state for the target is then the oscillator thermal state, truncated and scaled so that it is normalized. Our numerical studies confirm all of the claims made above: (i) our protocol is optimal, (ii) no more than $2N - 1$ auxiliary states are required for cooling resonators and qubits, and (iii) the best cooling is obtained just prior to $\tau = \pi/(2g)$. In Fig. 2(a) we show results for a two-level target with an of auxiliary size $M = 3$ ($\bar{n} = 0.5$), and we verified that $M = 4$ and $M = 5$ do no better. We also show two cases with target and auxiliary sizes $N = M = 4$, with $\bar{n} = 0.5$ and $\bar{n} = 0.1$. (With $\bar{n} = 0.1$, this gives a good approximation to an oscillator, as only the lowest four states are appreciably populated.) The inset shows cooling using our protocol up to the optimal time for $(N, M) = (2, 3)$, and the circles give numerical

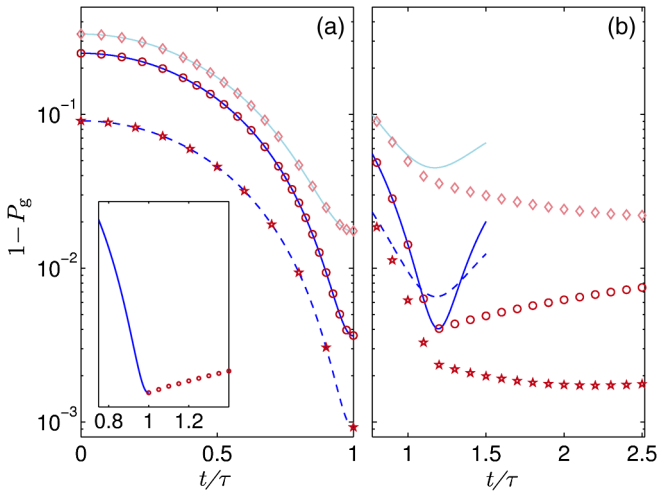

FIG. 2 (color online). The performance of our conjectured optimal cooling protocol compared against numerical optimization. The ground-state population is P_g, and $1 - P_g$ is shown versus time for systems of size N, cooled by an auxiliary of size M, with the control rate to damping rate ratio $\gamma/g = 0.01$, and initial thermal factors $\bar{n}$. The time scale $\tau = \pi/(2g)$. (a) Cooling using an ideal (undamped) auxiliary, in which our protocol is optimal. Dark line: $(N, M) = (2, 3)$, $\bar{n} = 0.5$; light line: $(N, M) = (4, 4)$, $\bar{n} = 0.5$; dashed line: $(N, M) = (4, 4)$, $\bar{n} = 0.1$; circles, squares, and diamonds: the corresponding results for numerical optimization. Inset: Numerical optimization beyond the optimal cooling time (see text). (b) Cooling the same systems as in (a), but the auxiliary is significantly damped with rate $\kappa = g$. Our protocol remains optimal for cooling a single qubit $[(N, M) = (2, 3)]$.

optimization past this time, confirming that optimal cooling is at $t \approx \pi/(2g)$. All these results use $\gamma/g = 0.01$.

Our analysis so far has assumed an ideal auxiliary system because we are interested in the absolute limit to cooling. Experimentally, however, nanoresonators are presently cooled via auxiliaries with significant damping, so the question of optimal protocols for this case is an interesting one. In Fig. 2(b) we perform optimization for an auxiliary with the damping rate $\kappa = g$. Remarkably, for a qubit our protocol remains optimal, and the performance is essentially unchanged. This also applies to resonators in the low-temperature limit. For larger N our protocol is no longer optimal, and the cooling is degraded as expected.

Having obtained numerical verification, we now calculate the final ground-state population for a harmonic oscillator and a qubit. To do this we use the linear versions of the quantum-jump stochastic master equations that are equivalent to the thermal master equations [18]. We exploit the fact that the dynamics is captured to first order in $\gamma\tau$ by one-jump trajectories; this technique can be applied to any dissipation operator [19]. We find that the maximum ground-state population is reached at $t = \tau$ (that the maximum is slightly before τ is a second-order effect). For a harmonic oscillator, taking $N \to \infty$, and thus also $M \to \infty$, the minimum population outside the ground state is

$$P_{\min} = \frac{\pi\gamma}{4g}\bar{n}\left(1 + \bar{n}\frac{(3+\bar{n})}{4(1+\bar{n})^2} + \bar{n}^2\frac{(3+\bar{n})}{2(1+\bar{n})^2}\right), \quad (3)$$

where g is the bound on the absolute values of the eigenvalues of the interaction H_I, and in general for a resonator it depends on $\bar{n}$ (see below), $\bar{n}$ is the average number of phonons or photons in the target at the ambient temperature, and the regime of validity is $\gamma(\bar{n}+1)/g \ll 1$. When $\bar{n}$ is small the approximate "cooling factor" is $\bar{n}/P_{\min} = 4g/(\pi\gamma) \gg 1$. We note that optomechanical sideband cooling uses an auxiliary resonator, with the linear coupling $H_I^{\text{osc}} = \tilde{g}(a + a^\dagger)(b + b^\dagger)$, where a, b are the target and auxiliary annihilation operators. For cooling a resonator the size of the state space is $N \sim \bar{n}$, giving $g \sim \tilde{g}$ for $\bar{n} \ll 1$ and $g \sim \tilde{g}\,\bar{n}$ for $\bar{n} \gg 1$. Substituting these into Eq. (3) gives $P_{\min} \sim \gamma\bar{n}/\tilde{g}$ for both regimes $\bar{n} \ll 1$ and $\bar{n} \gg 1$, which is consistent with previous results on the best cooling possible with optomechanical sideband cooling [6,7].

For a single qubit, the minimum achievable excited-state population is

$$P_{\min} = \frac{\pi\gamma}{4g}P_T\left(\frac{1 - P_T/4}{1 - 2P_T}\right), \qquad \frac{\gamma}{g}\frac{(1-P_T)}{(1-2P_T)} \ll 1, \quad (4)$$

with P_T the excited-state population at temperature T. For $P_T \ll 1$ the cooling factor is again $4g/(\pi\gamma)$.

The method developed here for finding optimal protocols is not limited to cooling, and can be used for a wide range of state-preparation problems. As an example, we use it to determine the minimal error probability for the preparation of a qubit in the target state $(|0\rangle + |1\rangle)/\sqrt{2}$, subject to decay at rate κ and dephasing at rate γ. The master equation is $\dot{\rho} = -(\kappa/2)\mathcal{D}(|0\rangle\langle 1|)\rho - \gamma(\rho - \sigma_z\rho\sigma_z)$. The minimal probability that the system is found outside the target state is [19]

$$P_{\min} = \frac{\gamma\pi}{8g} + \frac{\kappa\pi}{32g}(2 - 5/\pi). \quad (5)$$

In conclusion, we have provided a method to obtain optimal protocols for cooling or state preparation—with very high confidence—in the dual regimes of weak coupling to the control system, and control that is strong compared to the noise (high-fidelity control). It is hoped that the structural insights we have obtained will be useful in understanding optimal control protocols for cooling and other tasks in the strong coupling regime.

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