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Demon-like algorithmic quantum cooling and its realization with quantum optics

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Simulation of the low-temperature properties of many-body systems remains one of the major challenges in theoretical[1-3] and experimental[4-6] quantum information science. We present, and demonstrate experimentally, a universal (pseudo) cooling method that is applicable to any physical system that can be simulated by a quantum computer[7-9]. This method allows us to distil and eliminate hot components of quantum states like a quantum Maxwell's demon[10,11]. The experimental implementation is realized with a quantum optical network, and the results are in full agreement with theoretical predictions (with fidelity higher than 0.978). Applications of the proposed pseudo-cooling method include simulations of the low-temperature properties of physical and chemical systems that are intractable with classical methods.

From quantum field theories[1] to high-T_c superconductivity[2] and chemical reactions[3], quantum simulation[7–9] provides a unique platform for exploring a domain of science that goes beyond the applicability of classical computing methods. Modern low-temperature physics has advanced primarily due to the development of efficient cooling methods. The same is also true for quantum information science. Here, we focus on the problem of 'pseudo cooling', which aims to decrease the average energy of quantum states for quantum simulation (temperature does not need to be well-defined; Supplementary Section IB). In general, one needs to not only use physical cooling[12] to avoid decoherence[13], but also to be able to prepare states that have low entropy distributions in the energy eigenbasis of the system Hamiltonian being simulated[14,15].

Similar to many variational methods in quantum mechanics, states with average energies close to the ground-state energy would have a high overlap with the exact ground state, which can then be obtained with a high probability via the quantum phase estimation algorithm[9]. In quantum information science, solving ground-state problems is not only relevant to quantum simulation, but also provides resources for universal quantum computation[16,17].

An attractive approach for achieving cooling for spins (or qubits) is the heat-bath algorithmic cooling (HBAC) method[18]. The main idea behind HBAC is to reduce the entropy of qubits by unevenly distributing more entropy to one of the qubits, which can release the excess entropy to a heat bath through thermalization. The feasibility of HBAC has been demonstrated experimentally with NMR technology[4]. However, HBAC is not a universal method for cooling quantum many-body systems; it is primarily used for preparing polarized spins (that is, $|\downarrow\downarrow\downarrow \ldots \downarrow\rangle$) as initial states for quantum computation[19].

A different, yet closely related, approach[20,21] for quantum cooling is to engineer dissipative open-system dynamics to drive quantum states to the ground states of a simulated system. This dissipative open-system (DOS) approach is based on the simulation of Lindblad master equations, and has been shown to be robust[22] against simulation errors. A proof-of-principle demonstration has also been carried out using trapped ions[5]. Despite the advantages of the DOS approach, its range of application is limited. Practically, it is restricted to so-called frustration-free Hamiltonians[21], where the ground state should simultaneously minimize all local terms in the Hamiltonian.

In this work, we present a universal pseudo-cooling method, termed demon-like algorithmic cooling (DLAC), which is applicable to any physical system with Hamiltonian H_s that can be simulated by a quantum computer. Our method shares some features with the HBAC and DOS approaches. Similar to refs 4 and 23, we replace the requirement for an external heat bath with an ensemble of quantum states. With DOS, the quantum jump operators exploit the special structure of the frustration-free Hamiltonian to be simulated[20,21], which is not required in our case. This property makes our cooling method universally applicable to any physical Hamiltonian that can be simulated by a quantum computer.

We note that different cooling methods have advantages in different applications. For example, HBAC is more advantageous for ensemble quantum information processing[4], including highly mixed spin systems, and is also applicable to other scalable systems such as trapped ions[24]. Furthermore, HBAC is applicable for a heat bath at any non-zero temperature. DOS is potentially more efficient for preparing ground states of Kitaev's toric code model[22], and DLAC can be applied to enhance the probability of ground-state projection with the phase estimation algorithm[9]. Furthermore, pseudo cooling is also related to universal quantum computation. For example, the DOS approach can be implemented[21] in such a way that the fixed point (after a sufficiently long time) encodes the solution to a quantum computation problem. Therefore, in principle, the DOS approach can also be used to simulate the DLAC described in this work, except with some additional computational overhead.

The DLAC method works as follows. For any given Hamiltonian H_s and any input state, pure state $|\psi_{in}\rangle$ or mixed state ρ_{in}, the method guarantees that the energy $E \equiv \mathrm{Tr}(H_s\rho_{out})$ of output state ρ_{out} is less than (or equal to) that of the input state. Other than the system qubits, it requires only one extra ancilla qubit. This not only significantly reduces the computational resources required, but also makes the method more robust against noise and errors[22].

The core component of our method is the 'cooling module', which is formed by a simple quantum circuit (Fig. 1b). It consists

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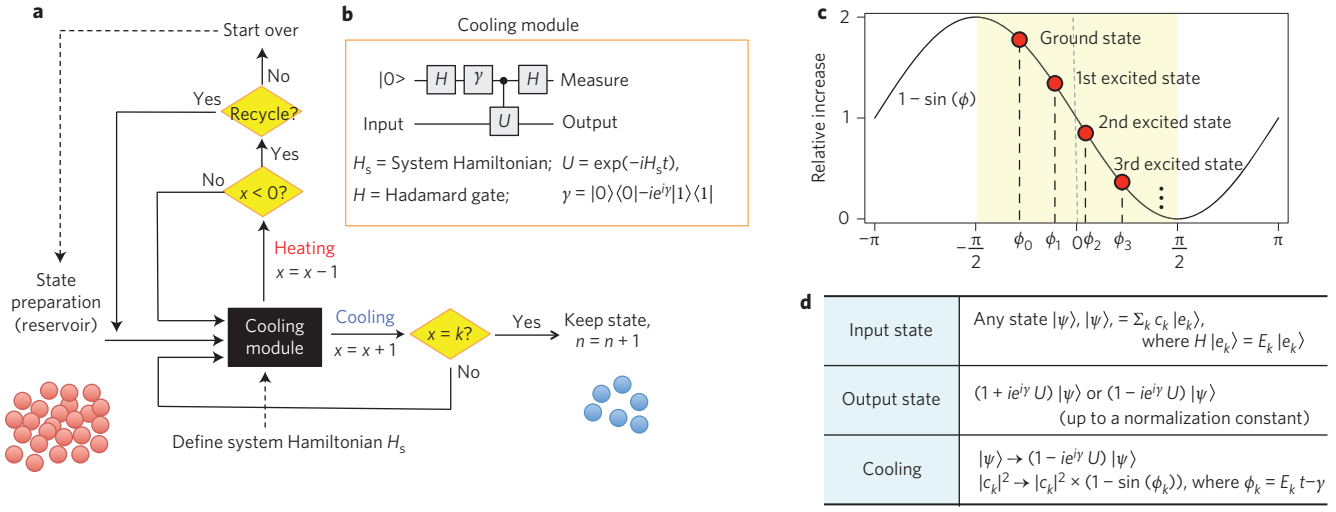

Figure 1 | Basic principle of the pseudo-cooling method. a, Logic diagram of the feedback cooling system. The cooling module produces two outcomes, correlated with heating and cooling. The measurement result can be mapped into the position x of a one-dimensional random walker. When the walker goes beyond its starting position $x = 0$ to the negative position $x = -1$, the particle is either rejected or recycled. **b**, The quantum circuit diagram of the cooling module. This includes a controlled evolution for time t and an energy bias parameter γ. **c**, The relative change in the population of the output state post-conditioned with a 'cooling' measurement result depends on the eigenenergy E_k: the lower the energy, the higher the gain. **d**, Summary of details (see also equation (1) and Supplementary Information).

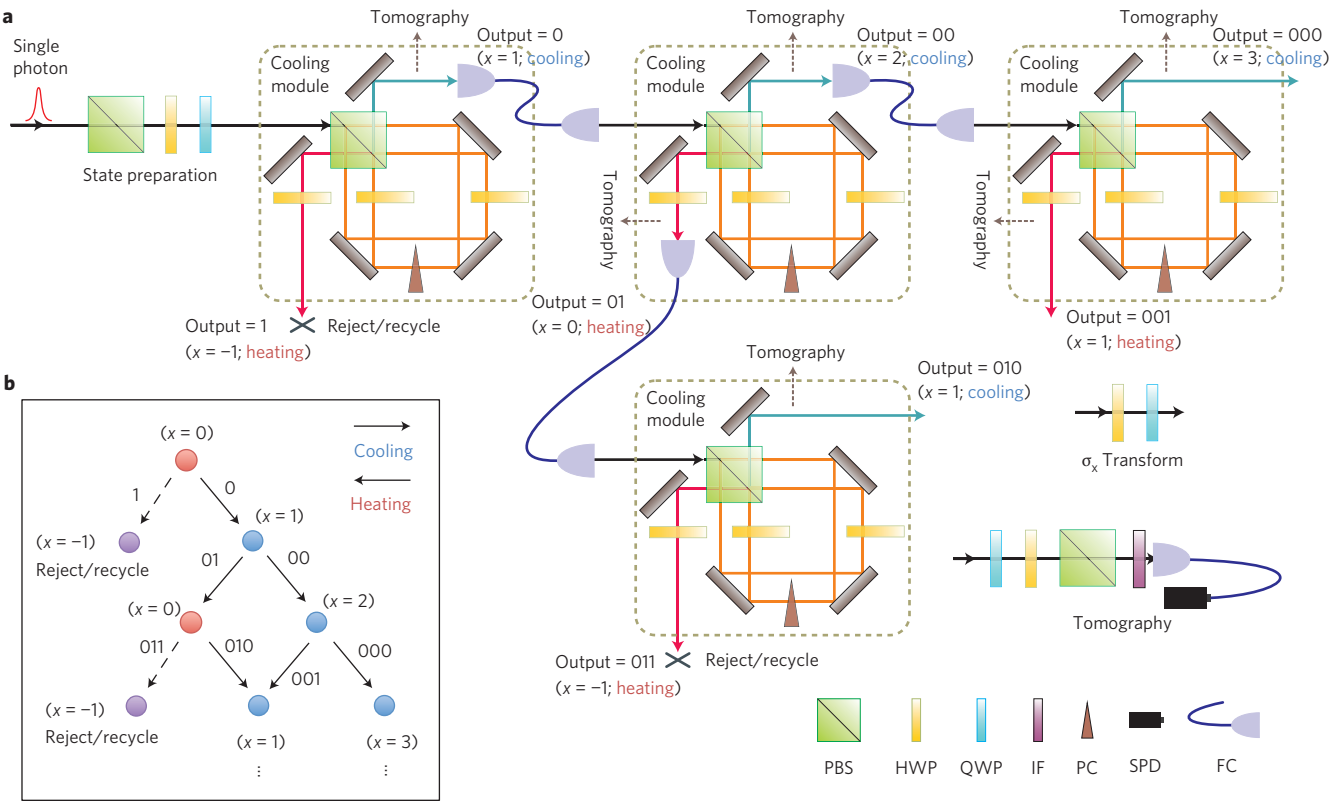

Figure 2 | Experimental details. a, The input photon state is prepared by a polarization beamsplitter (PBS), a half-wave plate (HWP) and a quarter-wave plate (QWP). The cooling module is a polarization-dependent Sagnac interferometer. Split by the PBS, the horizontal and vertical components of a polarized photon propagate along opposite paths within the interferometer. Two HWPs operate on the corresponding polarization components. The quartz plate compensator (PC) is used to compensate for the relative phase in the interferometer. These elements simulate the system Hamiltonian. Both paths are then recombined on the same PBS. The photons at output ports 0 and 1 represent the cases of cooling and heating, respectively. The photon proceeds to the next cooling module depending on the value of the position x of the random walker. The final quantum state is reconstructed using quantum state tomography, with the measurement bases defined by a QWP, HWP and PBS. The photon is detected by a single photon detector (SPD) equipped with a 3 nm interference filter (IF). When the simulated Hamiltonian is σ_x, a HWP with an angle of 22.5° and a tiltable QWP with a horizontal angle implement the σ_x transformation at the input and output ports. **b**, Sketch of the random walker evolution.

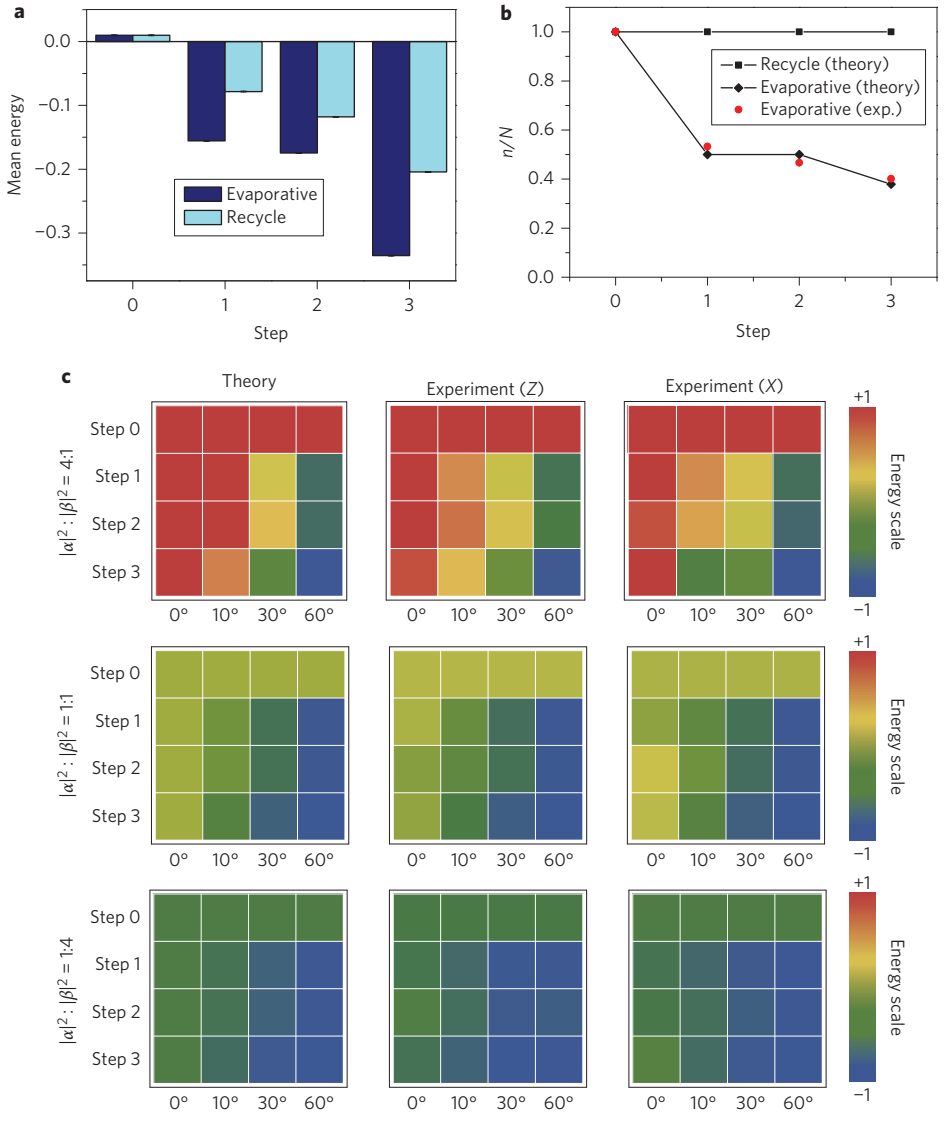

Figure 3 | Experimental results. a, Mean energies of the evaporative and recycling pseudo-cooling strategies for Hamiltonian σ_z, initial state $(|e\rangle + |g\rangle)/\sqrt{2}$, and bias angle $\theta = 10°$. **b**, Corresponding theory and experiment for n copies obtained out of N initial copies at consecutive steps. The total probability of the recycling algorithm is set to 1, correcting for experimental losses. **c**, Mean energies for three pseudo-cooling steps of the evaporative (non-recycling) strategy for different θ. Different maps correspond to theory and experiment for Hamiltonians σ_z (Z) and σ_x (X), and different initial states (step 0). Error bars in **b** represent the statistical distribution of experimental measurements; they are smaller than the symbols.

of an ancilla qubit initialized into the $|0\rangle$ state, a pair of Hadamard gates $H = (1/\sqrt{2})\left[(|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|\right]$, a phase gate $\gamma = |0\rangle\langle 0| - ie^{i\gamma}|1\rangle\langle 1|$ and a controlled unitary operation $U = \exp(-iH_s t)$, where H_s is the Hamiltonian to be simulated. We note that the unitary time evolution for most of the physical Hamiltonians can be simulated efficiently[7]. For any input state $|\psi_{in}\rangle$, the quantum circuit produces the following state (see Supplementary Section I for more details):

$$\Lambda_-|\psi_{in}\rangle|0\rangle + \Lambda_+|\psi_{in}\rangle|1\rangle \quad (1)$$

where $\Lambda_\pm \equiv (I \pm ie^{i\gamma}U)/2$.

The ancilla qubit is then measured in the computational basis $\{|0\rangle, |1\rangle\}$. The non-unitary operators $\Lambda_\pm$ play similar roles as the quantum jump operators in DOS[5,20–22] for describing the state evolution. Moreover, we found that the energy of the resulting states $\Lambda_-|\psi_{in}\rangle$ and $\Lambda_+|\psi_{in}\rangle$, after nomalization of the vector norms, is lower and higher, respectively, than that of the input state $|\psi_{in}\rangle$ (see Methods and Supplementary Section I). Consequently, the cooling module probabilistically projects any input state $|\psi_{in}\rangle$ (or ρ_{in} for mixed states) into either a higher-energy state $\Lambda_+|\psi_{in}\rangle$ (ancilla output $|1\rangle$) or a lower-energy state $\Lambda_-|\psi_{in}\rangle$ (ancilla output $|0\rangle$), with respect to the Hamiltonian H_s being simulated (Fig. 1c,d). Equation (1) represents the key element in our pseudo-cooling method.

The resulting photon in state $\Lambda_\pm|\psi_{in}\rangle$ will either be sent to another cooling module for further cooling, or restarted by a fresh photon, depending on the measurement outcome. We formulated this procedure as a feedback-control loop (depicted in Fig. 1a) and modelled the pseudo-cooling process as a one-dimensional random walk by keeping track of the measurement outcomes. Consider a random walker starting at position $x = 0$. If the measurement outcome is $|0\rangle$, then x is increased by 1. For $|1\rangle$ it is decreased by 1. When the random walker goes beyond the origin to the negative side ($x < 0$), the photon is replaced by a fresh photon. Net pseudo cooling is achieved by removing the hot components from the system in a way similar to Maxwell's demon[10].

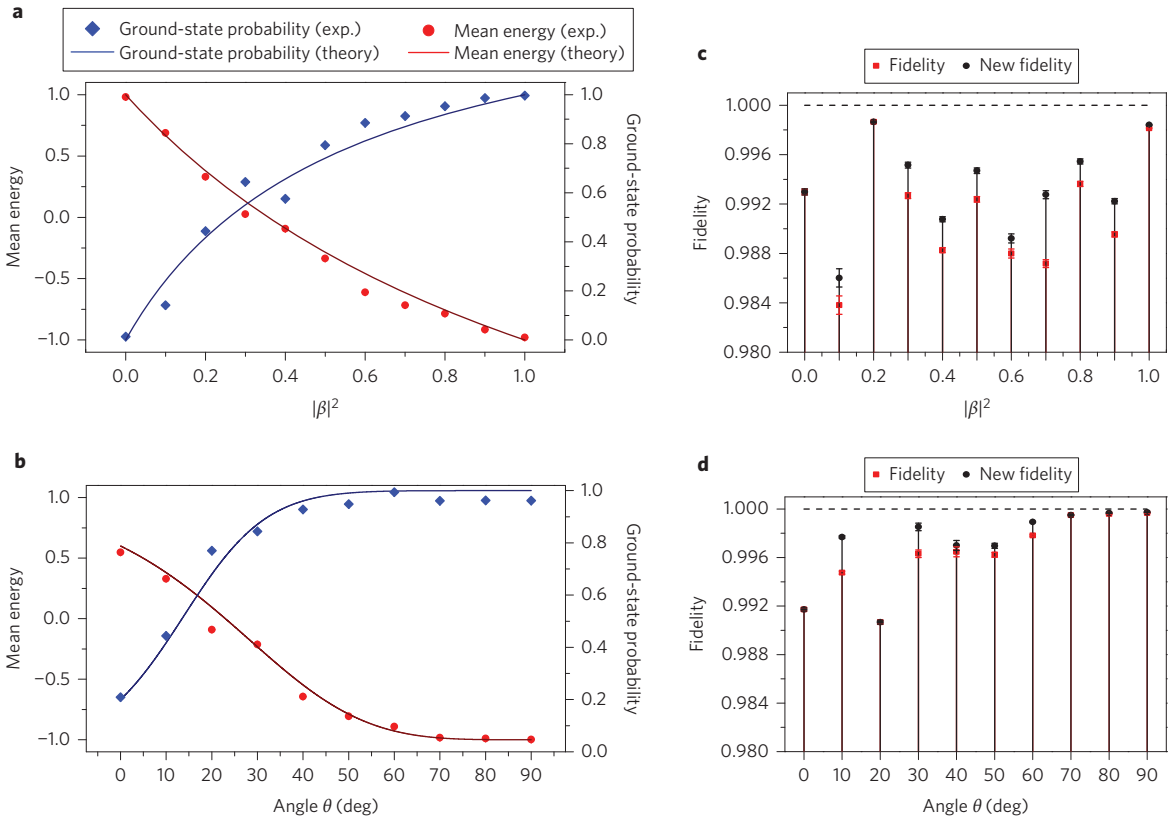

Figure 4 | Experimental results. a, Theoretical and experimental mean energy and ground-state probability after the third cooling step as a function of the initial ground-state overlap $|\beta|^2$. The evaporative strategy simulated the Hamiltonian σ_z with energy bias angle $\theta = 10^\circ$. **b**, Theoretical and experimental mean energy and ground-state probability after the third cooling step as a function of θ. The initial input state was $(2/\sqrt{5})|e\rangle + (1/\sqrt{5})|g\rangle$ ($|\alpha|^2 : |\beta|^2 = 4 : 1$) and the evaporative strategy simulated the Hamiltonian σ_z. **c**,**d**, Corresponding experimental and revised fidelities. Error bars correspond to the statistical distribution of experimental measurements.

In the following, we report a proof-of-principle demonstration of the quantum cooling method with an all-optical set-up (see, for example, ref. 25 for a recent review of photonic quantum simulation). We built a network of optical elements to connect four cooling modules (Fig. 2a) to implement multiple steps of pseudo cooling. This set-up is specifically designed for the polarization degrees of freedom of a single photon, that is, a qubit (see Supplementary Section IC for requirements for a scalable implementation). To illustrate the flexibility of the set-up, two different Hamiltonians H_s were simulated, namely Pauli's matrices,

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Although the Hamiltonians are relatively simple, the ground states are not assumed to be known. The logical Hilbert space of the system was encoded in the photonic polarization $\{|H\rangle, |V\rangle\}$. The goal of the experiment is to minimize the mean energy $\langle\sigma_z\rangle$ (or $\langle\sigma_x\rangle$) for any given initial state.

The which-path degree of freedom $\{|0\rangle, |1\rangle\}$ was used as the ancilla qubit in the quantum circuit (see equation (1)). The evolution operator $U(t) = \exp(-iH_s t)$ was simulated for a fixed period $t = \pi/2$. An energy offset, defined as

$$\theta \equiv \gamma + \pi/2 \qquad (2)$$

where γ is defined in Fig. 1b, was used as an adjustable parameter for characterizing the cooling efficiency.

Each of the cooling modules was realized by a polarization-dependent Sagnac interferometer (outlined with dashed lines in Fig. 2a). Similar, but not identical, structures[26,27] have been used for tasks related to quantum information processing. The quantum state $|\psi_{in}\rangle$ of the incident photon was prepared by a series of optical elements (Fig. 2a). The optical components inside the cooling module result in quantum logical operations[28] that are equivalent to that described in equation (1) (Supplementary Section IIIB). The photon leaving from one of the two output ports of the cooling module is in a superposition state (see equation (1)) containing both outcomes: heating $|1\rangle$ (red arrow) and cooling $|0\rangle$ (blue arrow). Subsequent detection of the two paths corresponds to a measurement in the ancilla qubit space, and will result in one of the two output states $\Lambda_\pm|\psi_{in}\rangle$.

The experimental results with multiple steps of pseudo cooling are summarized in Fig. 3. We compared the trade-off between the strategies with and without recycling of 'hot' copies. Figure 3a,b shows the theoretical and experimental results with initial input state $(|e\rangle + |g\rangle)/\sqrt{2}$, Hamiltonian σ_2 and energy bias angle $\theta = 10^\circ$. It is clear that the mean energy of the evaporative strategy decreases faster than that of the recycling strategy at the cost of a lower total yield. The colour-coded energy maps of Fig. 3c correspond to the evaporative strategy (that is, without recycling). We considered different initial input states $\alpha|e\rangle + \beta|g\rangle$ for Hamiltonians $H_s = \sigma_z$ and σ_x, and different proportions $|\alpha|^2 : |\beta|^2$ between the populations of the ground $|g\rangle$ and excited $|e\rangle$ states.

We systematically probed the mean energy $\langle H_s\rangle$ and the ground-state probability $P_g = \langle g|\rho_{exp}|g\rangle$ of the output states corresponding

to the cooling events after three steps, as shown in Fig. 4a,b. The mean energy decreases with increasing ground-state probability $|\beta|^2$ and energy bias θ. The output state approaches the ground state when θ is close to $\pi/2$, in good agreement with the theoretical prediction. Finally, the experimental fidelities F, defined by $F(\rho, \sigma) = \mathrm{Tr}\left(\sqrt{\rho}\sigma\sqrt{\rho}\right)^{1/2}$, are always larger than 0.983 and the fidelities after post-processing (see Methods) are even better (compare black and red data points in Fig. 4c,d).

To conclude, our simulation results show that our method of pseudo cooling for quantum simulation can be achieved experimentally with high fidelity. As the solution to classical[29] or quantum[30] computational problems can be encoded in the ground state of certain Hamiltonians, our pseudo-cooling method, like DOS[20,21], can potentially have applications beyond quantum simulation. The limitations of DLAC are discussed in the Methods.

Methods

Theoretical proof of the pseudo-cooling result. Here, we justify the claim in equation (1) that for any quantum state $|\psi_{\mathrm{in}}\rangle$ that is not an eigenstate of H_s, the state $\Lambda_-|\psi_{\mathrm{in}}\rangle$ ($\Lambda_+|\psi_{\mathrm{in}}\rangle$), after normalization, has energy $E = \langle H_s\rangle$ lower (higher) than that of $|\psi_{\mathrm{in}}\rangle$. To proceed, we performed an eigenvector expansion, which gives $|\psi_{\mathrm{in}}\rangle = \sum_k c_k|e_k\rangle$, where $|e_k\rangle$ are the eigenvectors of H_s, that is, $H_s|e_k\rangle = E_k|e_k\rangle$, and $c_k = \langle e_k|\psi_{\mathrm{in}}\rangle$. Consider $\Lambda_\pm|\psi_{\mathrm{in}}\rangle = \sum_k c_k\left(1 \pm ie^{-i\phi_k}\right)|e_k\rangle$, where $\phi_k \equiv E_k t - \gamma$. Note that the square norm of the amplitudes is $|c_k|^2(1 \pm \sin\phi_k)$. This means, that apart from an overall constant, each of the weights $|c_k|^2$ of the eigenvectors are scaled by a factor $(1 \pm \sin\phi_k)$. In Fig. 1c, within the range $|\phi_k| < \pi/2$, the function $1 - \sin\phi_k$ is monotonically decreasing. In other words, the lower the eigen-energy, the higher the weight gains, which results in a lower average energy, that is, pseudo cooling. A similar argument applies for the case of heating.

Pseudo cooling for universal quantum computation. The DOS approach can be modified[21] in such a way that quantum computation can be achieved through cooling. DLAC can also be applied for solving quantum-computation problems, provided that there is a finite energy gap above the ground state. It is now well known in the literature of adiabatic quantum computation that such a gap exists for all polynomial quantum circuits. Nevertheless, it is an open and interesting question whether one can always find an initial state with an overlap with the relevant ground state that scales polynomially. This result will imply that DLAC, like DOS, can also solve all BQP (bounded-error quantum polynomial time) problems efficiently.

Working mechanism of the cooling module. For the first cooling module, a single step of pseudo cooling is achieved if the measurement outcome is $|0\rangle$. To further extract energy from the system, multiple steps of pseudo-cooling events are needed. To proceed, four identical cooling modules were connected by optical fibres. The network of cooling modules (Fig. 2a) allowed us to implement multiple steps of pseudo cooling. The implementation was guided by following the random-walker diagram shown in Fig. 2b. Specifically, for any event where the photon emerges from the cooling (heating) exit of a cooling module, the random walk position x is increased (decreased) by 1. Across the boundary $x = -1$, for a range of parameters, the walkers have energy $\langle H_s\rangle$ higher than that of the initial state.

Limitations of DLAC. In this experiment, we demonstrated that DLAC is capable of cooling the polarization degrees of freedom (a two-level system) of photons efficiently. When applied to general high-dimensional ground-state problems, like many other existing quantum algorithms this method would take an exponential number of steps to approach the ground state. In fact, the ground-state problem belongs to the class of QMA (Quantum Merlin Arthur), which covers the class of problems termed BQP, which can be solved efficiently with a quantum computer. If there is any quantum algorithm that can solve all problems in QMA efficiently, this implies that QMA = BQP, which should be a result comparable with the famous problem—whether NP equals P or not. However, whether QMA equals BQP or not is still an intriguing open question. Nevertheless, we believe our cooling method is applicable to problems in physics and chemistry with symmetry and structure. For example, by using a classical solution such as the coupled-cluster method as an input state, the ground-state fidelity can be enhanced with our cooling method—the probability for projecting out the exact ground state using the phase estimation algorithm is increased.

Error analysis. In our experiment, the statistics of each count were considered to follow a Poisson distribution, and the error bars were estimated from the standard deviations of the values, calculated using the Monte Carlo method. The revised fidelities in Fig. 4c,d were obtained by mapping each experimental density matrix (obtained using maximum likelihood) to its eigenvector with the highest eigenvalue. This corrected isotropic (depolarizing) noise.

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Author contributions

M.-H.Y. and A.A.-G. are responsible for the main theoretical idea behind the pseudo-cooling method. S.B. performed detailed analysis on the scaling behaviour of the pseudo-cooling method. M.-H.Y. drafted the preliminary experimental proposal, which was put forward by Z.-W.Z. and C.-F.L. The detailed experimental procedures were designed and carried out by J.-S.X., assisted by X.-Y.X. The experiment was supervised by C.-F.L. and G.-C.G. All authors contributed to writing the manuscript and discussed the experimental procedures and results.

Additional information

Supplementary information is available in the online version of the paper. Reprints and permissions information is available online at www.nature.com/reprints. Correspondence and requests for materials should be addressed to C.F.L. and A.A.G.

Competing financial interests

The authors declare no competing financial interests.

CORRIGENDUM

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In the version of this Letter originally published online and in print, the affiliation of Sergio Boixo was incorrectly given. He is affiliated with the Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138, USA. This has now been corrected in the HTML and PDF versions of this Letter.