Quantum technologies require pure states, which are often generated by extreme refrigeration. Heat-bath algorithmic cooling is the theoretically optimal refrigeration technique: it shuttles entropy from a multiparticle system to a thermal bath, thereby generating a quantum state with a high degree of purity. Here, we show how to surpass this hitherto-optimal technique by taking advantage of indefinite causal order. Our protocol can create arbitrary numbers of pure quantum states without any residual mixedness by using a recently-discovered device known as a quantum switch, thereby fulfilling the dream of algorithmic cooling.

**Introduction.**—Quantum technologies promise dramatic improvements in computation, communication, metrology, and more. The vast majority of protocols require access to pure quantum states, which are typically provided by extreme refrigeration of mixed quantum states, but refrigeration has intrinsic limits and cannot be applied in all physical scenarios. To wit, cooling of trapped-ion and nuclear-magnetic-resonance systems, among others, will always leave some residual mixedness that degrades the purity of the quantum states [1–3].

Heat-bath algorithmic cooling (HBAC) was introduced as a method for simultaneously cooling a large ensemble of qubits, the most basic building blocks of quantum technologies. By serially replacing one of the qubits with one that was in thermal equilibrium with a large heat bath and performing a “compression” transformation on the qubits, as depicted in Fig. 1(a–b), entropy can be shuttled to the bath to cool the multi-qubit system [1–3]. This idea has been comprehensively investigated [4–12] and experimentally demonstrated [13, 14].

There is a fundamental limit to the cooling and therefore the purity that HBAC can achieve [4–6]. This was recently shown to stem from assumptions about the unitarity of transformations on the multi-qubit systems [11] and precludes any of the resulting states from ever being completely pure; instead, the optimal state is the probabilistic mixture given in Eq. (6). We here show that, by allowing for multiple unitary transformations to be applied in a superposition of their causal order, one can create completely pure states in a heralded fashion. This method simultaneously cools all of the qubits to their ground states, thereby shattering the limits that were previously imposed on HBAC.

Superpositions of causal order have become extremely relevant over the last decade. This phenomenon, known as indefinite causal order (ICO), has already been shown to break quantum limits in computation [15–18], communication [19–25], metrology [26–29], and thermodynamics [30–32], each of which were already known to outperform classical versions of the same protocols. ICO has been demonstrated in a number of groundbreaking experiments [33–41], many of which rely on a device known as a quantum switch to enable superpositions of the order in which unitary operations are applied to a system. This is a powerful new tool that is only beginning to be understood so, while it is remarkable to find yet another important application for ICO, it would not be surprising to discover that ICO has many more varied applications that we are only beginning to fathom.

In our first protocol, we replace the optimal unitary compression from HBAC with a controlled superposition of two unitaries that together achieve the original transformation, now depicted in Fig. 1c). Measuring the control in a superposition basis can then herald the creation of an unlimited number of completely pure qubits. We next explore and compare other purification protocols that incorporate ICO with different unitaries to achieve even faster purification, which can be optimized in terms of the temperature of the heat bath and other physical resources.

**Heat-bath algorithmic cooling (HBAC).—**The original techniques for HBAC have improved over the past few years. While the technique of Ref. [4] is optimal in that it achieves the ultimate cooling limit [5], it is state dependent and thus complex to implement. It was superseded by the technique of Ref. [8], which allows the ultimate cooling limit to be achieved without any knowledge of the state being cooled; we sketch this technique here (see Fig. 1a–b)).

The initial state to be cooled has \( n + 1 \) qubits in a state represented by the density matrix \( \rho \). Ultimately, the goal is to create the pure, ground state

\[
|g\rangle = |g\rangle \otimes \cdots \otimes |g\rangle, \quad \text{with } n+1 \text{ times}
\]

with the realistic goal being to create a state with as large of a probability as possible of being found in this state. We have access to a thermal bath at some temperature \( T \) from which we can extract thermalized qubits with density matrices

\[
\rho_{PR} = \frac{1}{\varepsilon} \begin{pmatrix} e^\varepsilon & 0 \\ 0 & e^{-\varepsilon} \end{pmatrix},
\]

while also being able to send any qubit to the bath such that it thermalizes into state \( \rho_{PR} \). Here, the subscript \( R \) stands for “reset,” the qubit is taken to be in the basis of ground and excited states \(|g\rangle\) and \(|e\rangle\) whose energies differ by \( \varepsilon k_B T > 0 \), \( \varepsilon = 2 \cosh k \), and we have assumed the bath to be sufficiently large such that it quickly thermalizes on a timescale more rapid than any other relevant to the rest of the protocol.
Particles to be purified/cooled

Reset

Heat bath

Unitary compression \( U \)

Controlled superposition of unitaries \( U_A \) and \( U_B \)

Heat bath

Particles to be purified/cooled

Reset

Unitary compression \( U \)

Controlled superposition of unitaries \( U_A \) and \( U_B \)

Heat bath

FIG. 1. Schematic of heat-bath algorithmic cooling (HBAC) augmented with indefinite causal order (ICO). Standard HBAC protocols repeatedly apply a and b; here, step b) is replaced by the ICO step c). a) One of a series of particles is replaced by a particle that has thermalized with an external heat bath. b) A unitary operation shuttles entropy from the particles on the left to those on the right, thereby cooling the particles on the left. c) A control qubit in a superposition state causes two unitaries \( U_A \) and \( U_B \) to be applied to the particles in a superposition of two orders. Measuring the control to be \( |+\rangle \) completely purifies all but one particle; measuring the control to be \( |--\rangle \) requires a repetition of the protocol. We define \(|\pm\rangle = (|0\rangle \pm |1\rangle) / \sqrt{2} \) throughout and the maximum number of allowed particles is unlimited and has negligible impact on the success probability.

First, whatever is occupying the position of the reset qubit is removed from the state and replaced with the state \( \rho_R \). This is mathematically represented by the operation (Fig. 1a)

\[
\rho \rightarrow \text{Tr}_R (\rho) \otimes \rho_R, \tag{3}
\]

where \( \text{Tr}_R \) is the partial trace removing the qubit in the reset position. Next, a unitary operation (Fig. 1b)

\[
U = \text{Diag}(1, \sigma_x, \ldots, \sigma_x, 1), \tag{4}
\]

where \( \sigma_x \) is a Pauli matrix and all of the off-diagonal entries are null, acts on the state to shift the larger probabilities like \( e^\varepsilon \) toward the \( |g\rangle \) part of the system and the smaller probabilities like \( e^{-\varepsilon} \) toward the opposite end. This "two-sort" unitary can be efficiently implemented [8]. The entire process is then repeated until, with a high degree of probability, the state reaches the theoretically coldest (most pure) state possible.

Only the diagonal elements of the density matrix are relevant to evaluating the success of this protocol. Denoting these by the \( 2^n+1 \)-component vector \( \mathbf{\lambda}' \) after the \( n \)th iteration of the protocol, \( \lambda'_1 \) represents the probability of finding the state to be \( |g\rangle \), \( \lambda'_i \) the probability of all of the qubits being in their ground states except for the reset qubit, and so on. Alternatively, we can focus on the probability distribution for the \( n \) qubits after ignoring the reset qubit, now denoted by the \( 2^n \)-component vector \( \mathbf{p}' \). In terms of these components, the removal of the reset qubit ensures \( p_k' = \lambda_{2k-1}' + \lambda_{2k}' (1 \leq k \leq 2^n) \), the addition of a thermal state leads to the intermediary probabilities \( \lambda_{2k}' = p_k e^\varepsilon / z \) and \( \lambda_{2k}' = p_k e^{-\varepsilon} / z \) (1 \( \leq k \leq 2^n) \), and the two-sort unitary rearranges the resulting vector to obey \( \lambda_{2k}' = \lambda_{2k+1}' \) and \( \lambda_{2k+1}' = \lambda_{2k}' \) (1 \( \leq k \leq 2^n) \). Overall, the probabilities are updated according to the rules \( \mathbf{p}^{n+1} = T \mathbf{p}' \), with transfer matrix

\[
T = \frac{1}{z} \begin{pmatrix} e^\varepsilon & e^\varepsilon & 0 & \cdots & 0 \\ e^{-\varepsilon} & 0 & e^\varepsilon & \cdots & 0 \\ 0 & e^{-\varepsilon} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-\varepsilon} & e^{-\varepsilon} \end{pmatrix}. \tag{5}
\]

Because \( T \) is almost a tridiagonal Toeplitz matrix, other than the first and last entries on its main diagonal, its eigenvalues can readily be computed. It has a single dominant eigenvalue corresponding to the hitherto-ultimate eigenstate

\[
\mathbf{p}^{\infty} = \frac{1 - e^{-2\varepsilon}}{1 - e^{-2(2^n)\varepsilon}} \begin{pmatrix} e^{-2\varepsilon} & e^{-4\varepsilon} & \cdots & e^{-(2^n-1)2\varepsilon} \end{pmatrix}^T, \tag{6}
\]

which is denoted by the superscript \( \infty \) because it is the ultimate final state toward which HBAC protocols evolve. This is the benchmark that HBAC protocols employing ICO are presently shown to beat; notably, none of the qubits is completely pure.

**Indefinite causal order (ICO).—** ICO leads to intriguing questions about the nature of causality [42–50]. One of its
offshoots is the development of a “quantum switch,” whose theoretical motivation [15, 51–55] and subsequent experimental implementation [33–41] have pushed the capabilities of quantum technologies well beyond what can be achieved without it [56]. We will show that a quantum switch is the only tool that we need in order to outperform HBAC protocols; it is likely that other protocols involving ICO will likewise be able to outperform HBAC protocols as well as other limits in quantum thermodynamics.

A quantum switch allows a single “control” state to control the order in which quantum operations are applied to a target state. For example, a two-switch can be represented by the unitary operator

$$U_{ICO} = |0\rangle_{\text{control}} \otimes |0\rangle_{B} U_{A} + |1\rangle_{\text{control}} \otimes U_{A} U_{B},$$

(7)

which leads to the evolution schematized in the centre of Fig. 1c: $U_{A}$ is applied before $U_{B}$ when the control state is $|0\rangle$ and $U_{B}$ is applied before $U_{A}$ when the control state is $|1\rangle$. We define the superposition states $|±\rangle = \frac{|0\rangle ± |1\rangle}{\sqrt{2}}$. If the control system is prepared in $|+\rangle$, the unitary is applied, and then the control is measured to be $|±\rangle$, the target system will evolve as

$$\rho \rightarrow \left( U_{A} U_{B} U_{B}^{\dagger} U_{A}^{\dagger} + U_{B} U_{A} U_{B}^{\dagger} U_{A}^{\dagger} \right) \pm U_{A} U_{B} \rho U_{A}^{\dagger} U_{B}^{\dagger} \pm U_{A} U_{B} \rho U_{B}^{\dagger} U_{A}^{\dagger} / 4.$$  

(8)

The first two terms are the convex combinations of the two orders of unitaries being applied, while the final two terms are unique interference effects stemming from ICO. These interference effects are what allow ICO to outperform standard quantum methods for a growing number of protocols.

ICO dramatically improves HBAC.— Putting together the pieces, we consider HBAC augmented with ICO (“HBAC+ICO” in Table I): we replace the unitary transformation $U$ with a pair of unitary transformations $U_{A}$ and $U_{B}$ whose order of application is controlled by a single auxiliary qubit (Fig. 1). We choose $U_{A}$ and $U_{B}$ such that both of the combined unitaries $U_{A} U_{B}$ and $U_{B} U_{A}$ independently lead to the transformation matrix $T$, with the interference effects arising only from ICO through Eq. (8). These are defined by

$$U_{A} = \text{Diag}(1, \sigma_{y}, \cdots, \sigma_{y}, 1),$$

$$U_{B} = \text{Diag}(1, \sigma_{y}, \cdots, \sigma_{y}, 1).$$

(9)

Because $\sigma_{y} \sigma_{y} = i \sigma_{x}$ and $\sigma_{y} \sigma_{y} = -i \sigma_{x}$, many cancellations result from Eq. (8). The probabilities now rearrange as $\lambda_{1}^{+1} = \lambda_{1}^{'+1} = (1 ± 1)/2$, $\lambda_{2k+1}^{+1} = \lambda_{2k+1}^{'+1} = (1 ± 1)/2$, and $\lambda_{2k}^{+1} = \lambda_{2k}^{'+1} = (1 ± 1)/2$ for $1 \leq k < 2^{n}$. When this quantum switch is added to the above HBAC protocol and the control is measured to be $|+\rangle$, the transfer matrix becomes

$$T_{+} = \frac{1}{z} \text{Diag}(e^{i\epsilon}, 0, \cdots, 0, e^{-i\epsilon}),$$

(10)

and similarly for $U_{B}$ with $\sigma_{z}$ replacing each $\sigma_{y}$, we find the probability of measuring the control to be $|+\rangle$ tends quickly toward $P = (1 - e^{-2\epsilon}) e^{i\epsilon}/z \approx \epsilon$ for moderate-to-large $n$. For completeness, we provide the transfer matrix for the case when the control is measured to be $|−\rangle$: 

$$T_{−} = T - T_{+}.$$  

(11)

If this result is obtained, the overall process can simply be repeated until the control qubit is measured to be $|+\rangle$, such that the success of the protocol is unequivocally known.

How can our protocol overcome what was previously thought to be a fundamental limit? The key is that, even though $U_{ICO}$ is unitary, our protocol involves a measurement step that allows us to avoid the assumptions of Ref. [11]. Adding a measurement step to standard HBAC would not help: since the final state is the probabilistic mixture given in Eq. (6), no measurement result will herald the rest of the qubits being pure. It is the combination of ICO with the measurement procedure that allows us to herald the creation of unlimited pure-qubit states.

Refining the idea.— The key to the advantage of ICO comes from the cancellations conferred by $U_{ICO}$ relative to the regular sorting unitary $U$. We have introduced these cancellations as replacing a single step in the HBAC protocol, but they can, in fact, replace the entire protocol. We shed light on some of the many avenues down which one can proceed after adding quantum switches to their toolbox.

First, consider an arbitrary $n+1$-qubit density matrix subject only to the quantum switch $U_{ICO}$ in Fig. 1e (“ICO alone” in Table I). Without the remainder of the HBAC protocol, we find the same transfer matrices as in Eqs. (10) and (11) but with all of the nonzero entries replaced by unity. In fact, we can consider how the coefficients of the entire state evolve, through $\lambda_{i}^{+1} = S \lambda_{i}^{'}$, with $S_{i}$ having the two eigenstates $|g\rangle$ and $|e\rangle$, and so the same protocol can be performed to fully purify $n$ of the qubits. Again, the process can be repeated indefinitely until the control qubit is measured to be $|+\rangle$ such that this result can be guaranteed with zero uncertainty. ICO alone can be used to implement algorithmic cooling, without recourse to shuttling entropy to and from an external heat bath!

Next, consider generalizing the superposed unitaries $U_{A}$ and $U_{B}$ by changing the locations of the Pauli matrices on their diagonals. If we choose

$$U_{A} = \text{Diag}(1, \cdots, 1, \sigma_{y}, \cdots, \sigma_{y})$$

(12)

and similarly for $U_{B}$ with $\sigma_{z}$ replacing each $\sigma_{y}$, we find the...
TABLE I. Comparing the resources required and probability of success of various purification schemes using ICO. There is no upper limit to the integer \( n \); "can be reduced to 1 if quantum nondemolition measurements are used, which may be considered as an auxiliary resource outside of HBAC and ICO.

| Scheme       | Bath          | Input pure qubits | Output pure qubits | \( P \) |
|--------------|---------------|-------------------|-------------------|--------|
| HBAC         | \( \varepsilon \) | 0                 | 0                 | 1      |
| HBAC+ICO     | \( \varepsilon \) | 1                 | \( n \)           | \( e \) |
| ICO alone    | none          | 1                 | \( n \)           | \( \lambda_1^0 + \lambda_{2n+1}^0 \) |
| ICO tree sort| none          | \( n^* \)         | \( n \)           | 1      |
| HBAC+ICO     | \( \varepsilon \) | 1                 | \( n + 1 - k \)   | \( 2^k e \) |

The transfer matrices

\[
S_+ = \text{Diag}(1, \ldots , 1, 0, \ldots , 0), \quad \text{with} \quad 2^n \times 2^n \times \text{times}
\]

\[
S_- = \text{Diag}(0, \ldots , 0, \sigma_x, \ldots , \sigma_x), \quad \text{with} \quad 2^n \times 2^n \times \text{times}
\]

Since these transformations hold for arbitrary permutations of the locations of the Pauli matrices on the diagonals of \( U_A \) and \( U_B \), this process can be repeated \( n \) times so that the resulting density matrix will be guaranteed to have \( n \) pure qubits and one mixed qubit, which we call the "ICO tree sort" method (Table I). However, this latter process requires \( n \) pure qubits to enable the \( n \) applications of the quantum switch, so it may not be physically useful! This latter process is only useful if the control qubit can be measured nondestructively such that a single pure qubit can be recycled for all \( n \) processes.

We thus see that applying ICO to upgrade HBAC protocols requires nuance. At least one pure qubit must be used to enable ICO, while the goal of HBAC is to generate a large number of pure qubits. It then follows that one can tailor an HBAC+ICO setup to optimize the number of pure qubits generated for a given number of input pure qubits, desired probability of success, and temperature of the heat bath, among other parameters.

For a given initial \( n+1 \)-qubit state, the ideal single-quantum-switch process uses \( U_A \) and \( U_B \) similar to that of Eq. (9):

\[
U_A = \text{Diag}(1, 1, \sigma_y, \ldots , \sigma_y), \quad \text{with} \quad 2^n \times \text{times}
\]

\[
U_B = \text{Diag}(1, 1, \sigma_z, \ldots , \sigma_z), \quad \text{with} \quad 2^n - 1 \times \text{times}
\]

Then, the ICO step alone yields \( n \) pure qubits after measuring or simply ignoring the first qubit, conditional on finding the control qubit to be \(|\rangle\rangle\). What is the probability of success for this protocol? It is \( \lambda_1^0 + \lambda_{2n+1}^0 \), the same as the probability of the original system to have all of the final \( n \) qubits be in their ground states. For a large number of qubits, this probability may be low, but the measurement can be repeated indefinitely until it is successful.

HBAC can help here ("HBAC+ICO" in Table I): after performing HBAC with a large number of qubits, the probability distribution tends toward \( p^\infty \), with which the probability of ICO success becomes double that of "HBAC+ICO":

\[
P = \lambda_1^0 + \lambda_{2n+1}^0 = P_1^\infty \approx 2\varepsilon, \quad \frac{1}{2^{n+1}} \ll \varepsilon \ll 1.
\]

One need only repeat the process \( m = O(1/\varepsilon) \) times in order to achieve any desired success probability \( P_{\text{des}} \), which can be used to make an unlimited number \( n \gg m \) pure qubits. Small \( \varepsilon \) corresponds to a hot heat bath and closely spaced energy levels \(|g\rangle\) and \(|e\rangle\), so this allows for significant refrigeration even with a hot bath! This works because the probability of success remains approximately constant with increasing \( n \). If, instead, one has access to a cold thermal bath, with large \( \varepsilon \), the probability of success tends to unity with a single protocol, so only one pure qubit need be supplied to generate an immense number \( n \) pure qubits.

In a regime with miniscule \( \varepsilon \), one can employ other tricks to improve the protocol. One can create a quantum switch with the unitaries from Eq. (14) replaced by unitaries with \( 2^k \) ones placed on the main diagonal before the remaining \( 2^n - 2^{k-1} \) Pauli matrices for some integer \( k \). Successfully measuring the control to be \(|\rangle\rangle\) and ignoring the final \( k \) qubits will then yield \( n + 1 - k \) pure qubits in their ground states ("HBAC+kICO" in Table I). Combined with the HBAC protocol, this will succeed with probability

\[
P = \frac{1 - e^{-2 \varepsilon 2^k}}{1 - e^{-2^{n+1} \varepsilon}} \approx 2^k \varepsilon \cdot 2^k \varepsilon \ll 1.
\]

Even with \( k \ll n \), the leading-order term \( 2^k \varepsilon \) can significantly hasten the convergence to a successful result. This now only requires \( m = O(2^{-k} \varepsilon^{-1}) \) trials to succeed in creating \( n + 1 - k \gg m \) pure qubits. Many such tricks can further expedite HBAC using ICO, thus establishing the import of quantum switches and related technologies to cooling protocols.

Concluding remarks.— We have shown that protocols incorporating indefinite causal order can dramatically outperform HBAC protocols that were previously thought to be optimal. Our protocols make use of a quantum switch to apply two unitary operations in a superposition of causal order in place of the single unitary in standard algorithmic cooling protocols, deterministically generating a vast number of completely pure quantum states. This solidifies the import of ICO in surpassing quantum limits that themselves already supersede classical bounds.

A few final comments pertain. First, one must be aware of the cost of doing a regular HBAC protocol to generate the probability distribution \( p^\infty \); this must be repeated \( m \) times to successfully generate the pure qubits. However, one can also calculate the effect that \( T_c \) has on \( p^\infty \), which may be negligible even when repeated a number of times, so one may only need to repeat the HBAC protocol a fraction of \( m \) times while implementing ICO \( m \) times. Second, HBAC protocols have recently been shown to potentially benefit from the presence of environmental noise [12]. This significantly improves the viability of all HBAC protocols, including the current proposal that augments HBAC with ICO. Third, if the ICO control is slightly
mixed, which can be evaded by a judicious choice of physical system for the control, the probability of creating $n$ pure qubits remains much higher than the corresponding probability using HBAC alone for realistic values of $\varepsilon$. Fourth, ICO has recently been linked to improvements in refrigeration [57–59] and thermometry [26]. Since purification is intimately linked to the amount of work that can be extracted from an ensemble of qubits, our purification protocol strongly supports the impact ICO may have on quantum thermodynamics. Finally, these results are readily extendable to multidisk systems while still only requiring a two-level control system to perform the ICO. Taken together, we are confident that ICO will continue to have a strong impact on quantum technologies including HBAC and beyond.

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