Equilibration to the non-Abelian thermal state in quantum many-body physics

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Quantum noncommutation was recently introduced into the following textbook statistical mechanics: Consider a small quantum system exchanging heat with a large bath via weak coupling. The small system equilibrates to a canonical ensemble [1].

\[ \rho_{\text{can}} := e^{-\beta H^S} / Z_{\text{can}}^S. \]  \hfill (1)

\(\beta\) denotes the bath’s inverse temperature, \(H^S\) denotes the system-of-interest Hamiltonian, and the partition function \(Z_{\text{can}}^S := \text{Tr}(e^{-\beta H^S})\) normalizes the state. If the system and bath exchange heat and particles, the system equilibrates to a grand canonical ensemble \(\propto e^{-\beta(H^S-\mu N^S)}\). The bath’s chemical potential is denoted by \(\mu\), and \(N^S\) denotes the system-of-interest particle-number operator. This pattern extends to electric charge and other globally conserved extensive quantities.

In statistical mechanics, a small system exchanges conserved charges—heat, particles, electric charge, etc.—with a bath. The small system thermalizes to the canonical ensemble, or the grand canonical ensemble, etc., depending on the charges. The charges are usually represented by operators assumed to commute with each other. This assumption was removed within quantum-information-theoretic (QI-theoretic) thermodynamics recently. The small system’s long-time state was dubbed “the non-Abelian thermal state (NATS).” We propose an experimental protocol for observing a system thermalize to the NATS. We illustrate with a chain of spins, a subset of which form the system of interest. The conserved charges manifest as spin components. Heisenberg interactions push the charges into the following textbook statistical mechanics: Conserved charges to charges fail to commute with each other.

Even if the system can thermalize, noncommutation invalidates some derivations of the thermal state’s form [7], as reviewed below.

QI theory was deployed to argue that a thermal state exists and has the form [7,9]

\[ \rho_{\text{NATS}} := e^{-\beta(H^S-\sum_{\alpha=1}^Q \mu_\alpha Q_\alpha^S)} / Z_{\text{NATS}}^S. \]  \hfill (2)

\(H^S\) denotes the system-of-interest Hamiltonian, \(Q_\alpha^S\) denotes the \(\alpha^{th}\) system-of-interest charge, the \(\mu_\alpha\)’s denote generalized chemical potentials, and the partition function \(Z_{\text{NATS}}^S := \text{Tr}(e^{-\beta(H^S-\sum_\alpha \mu_\alpha Q_\alpha^S)})\) normalizes the state. This non-Abelian thermal state (NATS) [2,7] has since spread across QI-theoretic thermodynamics [10,16].

This QI-theoretic thermodynamics is divorced from platforms and implementations: abstract, formal, and idealized. We regard it as describing the result of infinitely long thermalization at infinitely weak coupling.
Yet the NATS should be realizable under realistic conditions in condensed-matter, atomic-molecular, and high-energy systems. These fields have recently experienced a surge of interest in many-body thermalization. Therefore, we propose and numerically simulate an experimental protocol for observing a quantum many-body system thermalize to the NATS. Our protocol is suited to cold and ultracold atoms [17–28] superconducting qubits [29–31], trapped ions [32–34], nitrogen-vacancy centers in diamond [35], quantum dots [36], and perhaps nuclear magnetic resonance (NMR) [37]. To extend the NATS theory to finite times and coupling strengths, we propose initial steps toward a NATS many-body theory inspired by the eigenstate thermalization hypothesis (ETH) [38–40]. The point is that enhancing undergraduate statistical mechanics—the grand canonical ensemble—with noncommuting charges produces a thermal state that has never been observed. We observe such thermalization numerically, and we propose an experimental observation. The proposal shares the spirit of observations of the generalized Gibbs ensemble [41].

A brief review of the ETH, which informs our proposal, is in order. The ETH governs a chaotic quantum many-body system evolving under a nondegenerate Hamiltonian $H_{\text{tot}} = \sum_{m} E_m \rho^m$. Suppose that $H_{\text{tot}}$ conserves no nontrivial charges. Let $O$ denote a local observable that evolves to $O(t) := e^{-i H_{\text{tot}} t} O e^{-i H_{\text{tot}} t}$ in a time $t$. Let $\rho$ denote a whole-system state whose weights $\langle m | \rho | m \rangle$ peak sharply about some $E_m$. The observable’s expectation value approaches the canonical prediction:

$$\lim_{t \to \infty} \text{Tr}(O(t)\rho) \approx \text{Tr} \left( O e^{-\beta H_{\text{tot}}} / Z_{\text{can}}^t \right),$$

(3)

where $Z_{\text{can}}^t := \text{Tr}(e^{-\beta H_{\text{tot}}})$. The inverse temperature is defined through

$$\text{Tr} \left( H_{\text{tot}}^t \rho \right) = \text{Tr} \left( e^{-\beta H_{\text{tot}}} / Z_{\text{can}}^t \right).$$

(4)

The ETH features the whole-system Hamiltonian $H_{\text{tot}}$, rather than the $H^S$ in Eqs. (1) and (2).

Inspired by the ETH, we lay the foundations for a NATS theory within many-body quantum physics. The theory can be tested with an experiment of the following form. Consider a closed, isolated set of $N$ identical copies of a quantum system. We illustrate with a chain of qubits (quantum two-level systems), realizable with ultracold atoms (Fig. 1). One copy forms the system $S$ of interest. The other copies form an effective bath $B$. The dashed, blue arrows illustrate nearest-neighbor and next-nearest-neighbor interactions.

The whole system is prepared in a state $\rho$ in which each total charge, $Q_{\alpha}^t := \sum_{j=1}^N Q_{\alpha}^{(j)}$. The total Hamiltonian, $H_{\text{tot}} := \sum_{j=1}^N H^{(j)} + H^{\text{int}}$, is nonintegrable, to promote thermalization. The total Hamiltonian preserves each total charge: $[H_{\text{tot}}, Q_{\alpha}^t] = 0$. We illustrate $H_{\text{tot}}$ with nearest-neighbor and next-nearest-neighbor Heisenberg interactions.

FIG. 1: Setup for thermalization to the non-Abelian thermal state (NATS): We illustrate the general experimental setup with the spin-chain example proposed in Sec. I. The system $S$ of interest consists of $n = 2$ qubits. The other qubits form an effective bath $B$. The dashed, blue arrows illustrate nearest-neighbor and next-nearest-neighbor interactions.

The whole system is prepared in a state $\rho$ in which each total charge has a fairly well-defined value: Measuring any $Q_{\alpha}^t$ or $H_{\text{tot}}$ has a high probability of yielding a value close to the “expected value,” $S_\alpha$ or $E_\alpha$. $S_\alpha$ and $E_\alpha$ serve analogously to the grand canonical problem’s $N_\alpha$ and $E_\alpha$. The whole system then thermalizes internally for a long time under $H_{\text{tot}}$. A time linear in the system size suffices, according to numerics. A local observable $O$ of $S$ is then measured, as in ETH predictions.

We posit that the expectation value thermalizes to

$$\text{Tr} \left( O e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha Q_{\alpha}^t)} / Z_{\text{NATS}}^t \right),$$

(5)

rather than to the canonical prediction [3]. $S_\alpha$ and the $\mu_\alpha$’s, we posit, depend on $E_\alpha$ and the $S_\alpha$’s through

$$E_\alpha = \text{Tr} \left( H_{\text{tot}} e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha Q_{\alpha}^t)} / Z_{\text{NATS}}^t \right)$$

and

(6)

$$S_\alpha = \text{Tr} \left( Q_{\alpha}^t e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha Q_{\alpha}^t)} / Z_{\text{NATS}}^t \right).$$

We calculate $S_\alpha$ and the $\mu_\alpha$’s analytically in the spin-chain example. Existing ETH results—even those involving commuting charges—do not justify Eqs. (5) [3]. The noncommuting charges introduce into the energy spectrum degeneracies that could, a priori, lead to a different long-time state (Appendix A). We leverage the NATS theory to justify this prediction, and we test the prediction numerically in our spin-chain example.

En route to the thermodynamic limit, $S$ and $B$ grow large. The characteristic scale of $H^{\text{int}}$ remains constant, while the scale of $H^S$ grows. The scales’ ratio approaches zero. The whole-system quantities in Eq. (5) can be replaced with $S$ quantities:

$$\text{Tr} \left( O e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha Q_{\alpha}^t)} / Z_{\text{NATS}}^t \right)$$

$$\rightarrow \text{Tr} \left( O e^{-\beta (H^S - \sum_\alpha \mu_\alpha Q_{\alpha}^S)} / Z_{\text{NATS}}^8 \right).$$

(8)
Let $\rho_S$ denote the long-time state of S. If all S observables $O$ thermalize as in [8], S thermalizes to the NATS [2] of idealized QI-theoretic thermodynamics. Numerical simulations confirm that the state approaches the NATS prediction:

$$\rho_S \approx \rho_{\text{NATS}}.$$  \hspace{1cm} (9)

The rest of this paper is organized as follows. Section I illustrates our experimental proposal with a spin chain realizable with, e.g., ultracold atoms. Numerical simulations in Sec. II support the analytical predictions. Section III presents opportunities created by the introduction of noncommuting charges into many-body thermalization.

I. PROPOSAL FOR SPIN-CHAIN EXPERIMENT

We sketched a general experimental protocol in the introduction. Here, we illustrate with a spin chain. We detail the setup, preparation procedure, evolution, and readout.

Setup: Let S denote a system of $n > 1$ qubits. Consider a chain of $N$ copies of S (Fig. 1). A multidimensional lattice would suffice, as discussed before Eq. (10). The non-S copies form the effective bath, B. We index the qubits with $j = 1, 2, \ldots, N n$. Let $\sigma^{(j)}$ denote component $\alpha = x, y, z$ of the qubit-$j$ spin. The spin operators satisfy the eigenvalue equation $\sigma^{(j)}|\alpha\pm\rangle = \pm|\alpha\pm\rangle_j$. The chain has the total spin $\sigma^{(\text{tot})} = \sum_{j=1}^{Nn} \sigma^{(j)}$. Spins were applied in quantum thermodynamics to work extraction previously [5, 7, 9, 22, 43]. $H^{\text{tot}}$ must conserve each $\sigma^{(\text{tot})}$ while transferring subsystem charges between S and B. We construct such an $H^{\text{tot}}$ through physical reasoning. Let $\sigma^{(j)}_\alpha$ denote the raising and lowering operators for component $\alpha$ of the qubit-$j$ spin. For example, $\sigma^{(j)}_x = 1/2(\sigma^{(j)}_z \pm i \sigma^{(j)}_y)$. Rotating each side of this equation unitarily yields the raising and lowering operators for components $x$ and $y$. The two-site operator $J_\alpha(\sigma^{(j)}_+ \sigma^{(j+1)}_- + \text{h.c.})$ transports $\alpha$-charges between sites $j$ and $j + 1$ with frequency $J_\alpha$. The Hamiltonian must transport charges of all types, so we sum over $\alpha$. For the Hamiltonian to commute with each total charge, the $J_\alpha$'s must equal each other. A Heisenberg interaction results: $J \sum_{\alpha=x,y,z} (\sum_{j=1}^{Nn} \sigma^{(j)}_+ \sigma^{(j+1)}_- + \text{h.c.}) = \sum_{j=1}^{Nn} \sigma^{(j)}_x \sigma^{(j+2)}_x$.

The nearest-neighbor Heisenberg interaction is integrable. Nearest-neighbor interactions break integrability, as would a higher-dimensional lattice. We therefore choose for the spin chain to evolve under

$$H^{\text{tot}} = J \left( \sum_{j=1}^{Nn-1} \sigma^{(j)}_+ \sigma^{(j+1)}_- + \sum_{j=1}^{Nn-2} \sigma^{(j)}_x \sigma^{(j+2)}_x \right).$$  \hspace{1cm} (10)

Similar interactions have been realized with ultracold atoms [22, 28, 44], symmetric top molecules [45, 46], trapped ions [33], and NMR [37]. Furthermore, anisotropic interactions can often generate isotropic effective interactions [7]: The system is evolved under the original Hamiltonian, the $z$-axis is rotated into the $x$-axis, the system is evolved further, the new $x$-axis is rotated into the new $y$-axis, and then the system is evolved further.

Our interaction is weak: $H^{\text{int}}$ consists of the six $\vec{\sigma} \cdot \vec{\sigma}$ terms that link S to B. Hence the interaction energy $\sim 6J$. $H^{\text{S}}$ consists of the six bonds that act on just S. Hence S has energy $\sim J n$. The interaction-energy-to-S-energy ratio vanishes in the thermodynamic limit, as $N, n \to \infty$. As the interaction is weak, intuition from master equations [48, 49] predicts thermalization of S.

Preparation procedure: The grand canonical problem motivates our preparation procedure. Consider aiming to watch a small system thermalize to the grand canonical ensemble. The system-and-bath composite should be prepared with a well-defined total energy, $E^{\text{tot}}$, and total particle number, $N^{\text{tot}}$. If classical, the whole system occupies a shell in phase space. The shell’s width stems from measurement imprecision. If quantum, the total system approximately occupies a microcanonical subspace, an eigenspace shared by the total Hamiltonian and total particle-number operator [11, 50].

Let us translate this protocol into the noncommuting problem. One might aim to prepare the whole system with a well-defined $\sigma^{(\text{tot})}_\alpha$ for all $\alpha = x, y, z$. But the spin components fail to commute; they share no joint eigenspace. The microcanonical subspace was therefore generalized to an approximate microcanonical (a.m.c.) subspace, $\mathcal{M}$ [2]. In $\mathcal{M}$, every total charge has a fairly well-defined value $S^{\alpha}_\alpha$: Measuring any $\sigma^{(\text{tot})}_\alpha$ has a high probability of yielding a value close to $S^{\alpha}_\alpha$. $S^{\alpha}_\alpha$ serves similarly to the commuting problem’s $N^{\text{tot}}$. The probability and closeness were quantified in [7] and are reviewed below. The longer the spin chain, the more certain the measurement outcome can be.

We seek to prepare a whole-system state that satisfies three conditions: (i) Each total charge has a fixed mean: $\langle \sigma^{(\text{tot})}_\alpha \rangle = S^{\alpha}_\alpha$. (ii) Each total charge has a subextensive standard deviation:

$$\sqrt{\langle (\sigma^{(\text{tot})}_\alpha)^2 \rangle - \langle \sigma^{(\text{tot})}_\alpha \rangle^2} < N n.$$

(iii) The state is not equivalent, via any $H^{\text{tot}}$-preserving transformation, to any U(1)-symmetric state. This condition reduces our protocol’s similarity to well-known thermalization in the presence of U(1) symmetry. For further discussion about the processes’ inequivalence, see App. A. We exhibit three protocols that satisfy conditions (i)–(iii).

In the first protocol, a fraction $S^{\alpha}_\alpha/(N n)$ of the qubits are prepared in $|\alpha+\rangle$, for each of $\alpha = x, y, z$. The $\langle \sigma^{(\text{tot})}_\alpha \rangle$’s satisfy property (i) because, e.g., $|z+\rangle$ contributes zero quanta to $\langle \sigma^{z}_{x} \rangle$ and $\langle \sigma^{z}_{y} \rangle$. The state satisfies property...
(ii) because every $\langle \sigma^{\alpha \text{tot}} \rangle$ has a subextensive standard deviation in every short-range-correlated state (App. B). Second, spin-coherent states are known to satisfy properties (i) and (ii) \[5\].

To motivate the third protocol, we return to the grand canonical problem. One can fix $E^{\text{tot}}$ and $N^{\text{tot}}$ by measuring the total energy, then the total particle number. One could analogously, in the noncommuting problem, measure $H^{\text{tot}}$, then $\sigma^{\alpha \text{tot}}$, then $\sigma^{\beta \text{tot}}$, then $\sigma^{\gamma \text{tot}}$. But the $y$ and $z$ measurements would disturb the $x$ and $y$ components. The projective measurements must be “softened.” We define a soft measurement as having two properties, (a) peaking and (b) mild disturbance: (a) Suppose that $\sigma^{\alpha \text{tot}}$ is measured softly, yielding outcome $\tilde{S}_\alpha$. Suppose that $\sigma^{\alpha \text{tot}}$ is then measured strongly. The outcome must have a high probability of lying close to $\tilde{S}_\alpha$. (b) Suppose that $\sigma^{\alpha \text{tot}}$ is measured strongly, then some other $\sigma^{\beta \text{tot}}$ is measured softly, and then $\sigma^{\gamma \text{tot}}$ is measured strongly again. The final measurement must have a high probability of yielding the first measurement’s outcome. The soft measurement must scarcely disturb $\sigma^{\alpha \text{tot}}$.

We formalize soft measurements in App. C using a positive operator-valued measure (a mathematical model for a generalized measurement \[52\]) with a binomial envelope. Similar measurements have been implemented via weak coupling of system and detector \[53\, Eq. (22)] [53]. Appendix D reconciles Ineq. (11) with the a.m.c. subspace’s original definition \[7\].

**Evolution:** The whole system has been prepared in some state in an a.m.c. subspace $\mathcal{M}$. The chain is now evolved under $H^{\text{tot}}$. Numerical simulations imply that a time $\sim Nn/J$ suffices for distinguishing the NATS from the canonical prediction. The interaction hops spin quanta between sites. The evolution is intended to prepare the chain in an a.m.c. ensemble, the noncommuting analog of the microcanonical ensemble: Let $P_M$ denote the projector onto $\mathcal{M}$. The a.m.c. ensemble is defined as $P_M/\text{Tr}(P_M)$ \[7\]. Tracing out the bath from $P_M/\text{Tr}(P_M)$ was proved analytically to yield a system-of-interest state close to the NATS \[7\].

**Readout:** We aim to test that analytical prediction experimentally. Let $\rho_S$ denote the long-time state of $S$. We posit that most local observables $O$ end with expectation values given by the NATS prediction \[5\], rather than the ETH prediction \[3\]. Equations (6) and (7) determine $\beta$ and the $\mu_\alpha$’s.

We calculate $\beta$ and the $\mu_\alpha$’s analytically for the spin chain in App. E. We assume that the system is hot and the effective chemical potentials are small. Loosely speaking,

$$\sqrt{Nn} |\beta| J \sqrt{\frac{Nn}{\alpha} \sum_\alpha \mu^2_\alpha |\beta|} \frac{\beta^2}{J} \sum_\alpha \frac{\mu^2_\alpha}{J} \ll 1. \quad (12)$$

More-precise forms for the constraints depend on boundary conditions and appear in App. E. The inverse temperature evaluates to

$$\beta = \frac{-E^{\text{tot}}}{3(2Nn - 3J)J} + O_2. \quad (13)$$

$O_2$ stands for “terms of second order in the small parameters in \[12\].” The effective chemical potentials evaluate to

$$\mu_\alpha = -\frac{3(2Nn - 3J)}{Nn} \frac{S_\alpha J^2}{E^{\text{tot}}} + O_2. \quad (14)$$

In the thermodynamic limit, $H^{\text{int}}$ drops out of the prediction \[3\], as discussed in the introduction. If all $S$ observables $O$ have NATS expectation values, $S$ thermalizes to the NATS state \[2\]. Outside the thermodynamic limit, noncommutation may prevent $\rho_S$ from reaching $\rho_{\text{NATS}}$ precisely \[7\]. The distance between the states was quantified with the relative entropy,

$$D(\rho_S||\rho_{\text{NATS}}) = \log(\rho_S \log \rho_S - \log \rho_{\text{NATS}}). \quad (15)$$

Logarithms are base-e throughout this paper. The relative entropy quantifies the accuracy with which $\rho_S$ can be distinguished from $\rho_{\text{NATS}}$, on average, in a binary hypothesis test \[52\]. The relative entropy \[15\] was predicted to decline as the number $N$ of systems grows \[7\]:

$$D(\rho_S||\rho_{\text{NATS}}) \leq \frac{\text{const.}}{\sqrt{N}} + \text{const.} \quad (16)$$

This scaling can be checked with quantum state tomography \[14\] in the finite-size experiments feasible today. We detail the tomographic process in App. F. Numerical simulations point to a scaling close to \[16\] (Sec. II). The constant term in \[16\] comes from the charges’ noncommutation. The constant depends on the parameters that quantify how much the definition of “microcanonical subspace” is relaxed to include $\mathcal{M}$. The larger the whole system, the better the $(Q^{\alpha \text{tot}}/N)$’s commute, so the less the definition needs relaxing, so the greater the probability that some $\mathcal{M}$ corresponds to a smaller constant.

**II. NUMERICAL SIMULATIONS**

We numerically simulated the experimental protocol via direct calculation. The spin chain’s length varied from $Nn = 6$ to 14 qubits. The first two qubits served as $S$, without loss of generality due to periodic boundary conditions.

We followed the first state preparation protocol in Sec. I. The first six qubits were prepared in $|x+\rangle|z+\rangle|x-\rangle|z-\rangle|x-\rangle|z+\rangle$; and the rest of the qubits, in copies of $|z-\rangle|z+\rangle$. Hence the total charges had the expectation values $S_x = -1$, $S_y = 0$, and $S_z = 1$.

The state evolved under the Hamiltonian \[10\] for a time $t = 2^{Nn}$, wherein $J = 1$. The exponential time sharpens the distinction between the NATS and canonical predictions. However, a time $t \sim Nn$ suffices. Usually, when simulating charge-conserving evolution, one
represents the Hamiltonian as a matrix relative to an eigenbasis shared with the charges. Such an eigenbasis does not exist here, due to the charges’ noncommutation.

Figure 2 shows the relative entropies. The blue dots show $D(\rho_S\|\rho_{\text{NATS}})$; the red squares, $D(\rho_S\|\rho_{\text{can}})$; and the green triangles, $D(\rho_S\|\rho_{\text{GC}})$. The NATS theory predicts $\rho_S$ with greater accuracy, which grows with the spin chain. The dotted lines show the best fit to any function of the form of the right-hand side of Eq. (16), $-0.128 + 0.336N^{-1/2}$. This function fits with a standard deviation of 0.010 and an error of 0.022. In App. C we study robustness with respect to experimental errors caused by anisotropic couplings.

III. DISCUSSION

We have formulated and simulated an experimental protocol for thermalizing a quantum many-body system to the NATS. The protocol suits ultracold atoms, trapped ions, quantum dots, nitrogen-vacancy centers, and perhaps NMR. This work initiates a bridge from the abstract, idealized NATS theory of QI-theoretic thermodynamics to many-body physics: We introduce noncommutation—a basic feature of nonclassicality—of charges into condensed-matter and AMO physics. Extensions to high-energy physics beg to be realized.

Condensed-matter, AMO, and high-energy physics have recently witnessed the development of toolkits for studying many-body thermalization: quantum-simulator experiments [25, 29, 32, 33, 37], the ETH [38–40], random unitary circuits [57, 60], the generalized Gibbs ensemble (GGE) [41, 55, 56], and out-of-time-ordered correlators [61]. These frameworks can now be leveraged to explore noncommutation’s effects on thermalization. Constraining dynamics, noncommutation might slow the transport of energy, information, and/or charges. Hence noncommutation might enhance storage and memory. Additionally, noncommutation underlies quantum error correction, quantum cryptography, and other applications. Noncommutation might advance information processing in materials. Furthermore, group theory structures high-energy physics. Particle physics and string theory might involve non-Abelian groups that give rise to NATS physics.

The thermodynamic limit, too, merits study. We focus on the finite system sizes $N$ realizable experimentally. But Fig. 2 shows that, as the whole system grows, the canonical prediction’s accuracy grows. Whether the NATS prediction outperforms the canonical in the limit as $N \rightarrow \infty$ offers a theoretical opportunity for investigation.

So do degeneracies. The ETH describes nondegenerate Hamiltonians. Conserved charges introduce degeneracies, which can affect thermodynamic ensembles. We address degeneracy through the microcanonical lens of [7]: Noncommutation can prevent the charges from sharing an eigenspace. No degenerate microcanonical subspace necessarily exists. The microcanonical subspace was therefore generalized to the a.m.c. subspace in [7]. We have proposed protocols for preparing a global system in an a.m.c. state. This QI-thermodynamic approach to degeneracy should be complemented with a many-body-
physics approach informed by ETH studies.

We close by illuminating the NATS from two many-body angles: We contrast the NATS with the GGE and repurpose an insight about the ETH. The GGE is an ensemble to which quantum systems equilibrate if extensively many nontrivial charges are conserved. Our prediction lies outside existing GGE studies for three reasons. First, GGE studies have not emphasized noncommutation. Second, GGE Hamiltonians are integrable; ours is not. Third, GGE charges tend not to equal sums of local charges. We demand the extensivity present in the textbook problem reviewed in the introduction. This demands highlighting how adding noncommutation to well-known statistical mechanics generates new physics.

Deutsch’s original ETH paper offers another lens through which to view our NATS protocol. The ETH describes a closed quantum many-body system’s thermalization to a canonical state. Quantum systems were known to thermalize to the canonical state by exchanging heat with external baths. Did the ETH not there-known to thermalize to the canonical state by exchanging to a canonical state. Quantum systems were described a closed quantum many-body system’s thermalization. Different mechanisms drive the two thermalizations, as in Deutsch’s argument. A classical external field thermalizes spins to \( \rho_{\text{triv}} \). Exchanges of noncommuting charges within a closed, isolated quantum system thermalizes spins to the NATS. As ETH thermalization studies, so does NATS thermalization. NATS thermalization arguably demands more, highlighting nonclassical noncommutation.

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**Appendix A PROTOCOL’S INEQUIVALENCE TO THERMALIZATION UNDER A HAMILTONIAN THAT HAS ONLY U(1) SYMMETRY**

One might worry that our protocol’s final state could be predicted without the NATS theory, that the NATS adds nothing to our knowledge of thermalization. *Prima facie*, the prediction seems to require knowledge of only the ETH and thermalization under U(1)-symmetric Hamiltonians. The latter thermalization has been studied in, e.g., [59, 60]. A U(1)-symmetric qubit Hamiltonian conserves \( \sigma_z \). The Hamiltonian is equivalent, via a Jordan-Wigner transformation, to a Hamiltonian that conserves particle number. Hence systems thermalize to the grand canonical ensemble under U(1)-symmetric evolution. This thermalization, we show, is inequivalent to our protocol’s thermalization: Justifiably predicting our protocol’s final state requires knowledge of the NATS. Afterward, we present three more reasons for the inequivalence of thermalization to the NATS and thermalization under a U(1)-symmetric Hamiltonian: First, microscopic dynamics distinguish the two thermalization processes. Second, thermalization to the NATS is inequivalent to thermalization to the grand canonical ensemble just as thermalization to the grand canonical state is inequivalent to thermalization to the canonical state. Third, our thermalization protocol and thermalization to the grand canonical state lead to thermal states whose group-theoretic properties differ.

First, we elucidate why our protocol’s final state appears predictable with just knowledge of the NATS and of thermalization under U(1)-symmetric Hamiltonians. Imagine learning our protocol’s initial state, \( \rho \), and Hamiltonian, \( H^{\text{tot}} \). Imagine having to predict the final state’s form without knowing the NATS theory. One might reason as follows: \( H^{\text{tot}} \) has SU(2) symmetry. \( \sigma_x^{\text{tot}}, \sigma_y^{\text{tot}} \) and \( \sigma_z^{\text{tot}} \) generate SU(2). Hence the evolution conserves \( \langle \sigma_z^{\text{tot}} \rangle = \text{Tr}(\rho \sigma_z^{\text{tot}}) \) for all \( \alpha = x, y, z \). The expectation values form a vector \( (\langle \sigma_x^{\text{tot}} \rangle, \langle \sigma_y^{\text{tot}} \rangle, \langle \sigma_z^{\text{tot}} \rangle) \equiv \hat{r} \). The coordinate system can be transformed such that \( \hat{r} \) coincides with the new \( z \)-direction, \( \hat{z} \). The transformation conserves \( H^{\text{tot}} \). In this reference frame, only \( \langle \sigma_z^{\text{tot}} \rangle \neq 0 \). Furthermore, \( \langle \sigma_z^{\text{tot}}(t) \rangle \) remains constant. The thermalization therefore appears, *prima facie*, identical to thermalization under a U(1)-symmetric Hamiltonian. One might therefore predict that the system of interest thermalizes to a grand canonical state in this reference frame. Knowing the ETH, one might predict Eq. [5], wherein \( \sum_{\alpha} \mu_{\alpha} Q_{\alpha} = \mu_z \sigma_z^{\text{tot}} \), despite misrepresenting the microscopic dynamics (see below). One could extrapolate the ETH to reconstruct the NATS prediction. Without the NATS theory, however, this prediction would have even less justification than most ETH claims. (The ETH remains a hypothesis. Analytical support for the ETH remains
under construction.)

The ETH is justified when the initial state’s support lies on a small microcanonical window of energy levels. Consider the extension of the ETH to the grand canonical ensemble. The Hamiltonian shares an eigenbasis with the particle-number operator. The extension is justified when the initial state’s weight lies on a small microcanonical window of shared eigenstates. Now, consider extending the ETH to thermalization under a Hamiltonian that conserves noncommuting charges $Q^\text{tot}_\alpha$. One would naively expect the extension to be justified when the initial state’s support lies on a small microcanonical window of eigenstates shared by $H^\text{tot}$ and all the $Q^\text{tot}_\alpha$’s. Earlier studies of thermalization in the presence of $U(1)$ symmetry would support the extension. But the $Q^\text{tot}_\alpha$’s do not necessarily share eigenstates, as they fail to commute. Hence an extension of the ETH seems impossible to justify...unless the notion of a microcanonical subspace is generalized to an approximate microcanonical subspace. This generalization forms a cornerstone of the NATS theory [7]. Hence the NATS theory is necessary for justifiably predicting the state to which our system thermalizes. This paper shows that the prediction is accurate for finite-size spin chains evolving under Eq. (10).

NATS thermalization is inequivalent to thermalization under a $U(1)$-symmetric Hamiltonian for three more reasons. First, under $U(1)$ symmetry, just two quantities hop between subsystems: energy and quanta of one component of angular momentum. Quanta of all three components of the angular momentum—charges that fail to commute with each other—hop during thermalization to the NATS. One misrepresents the microscopic dynamics when attempting to reduce NATS thermalization to thermalization under a $U(1)$-symmetric Hamiltonian.

The attempt’s failure parallels the failure to reduce grand canonical thermalization to canonical thermalization. The grand canonical state is $\propto \exp(\beta H - \mu N)$, wherein $H$ denotes a Hamiltonian, $N$ denotes a particle-number operator, and $\mu$ denotes a chemical potential. One can define an effective Hamiltonian $\tilde{H} := H - \mu N$. The grand canonical state will look identical to a canonical state, $\propto \exp(\beta \tilde{H})$. But this definition cannot reduce grand canonical physics to canonical physics. During thermalization to the canonical state, subsystems exchange only energy. During thermalization to the grand canonical state, subsystems exchange energy and particles. The very existence of the name “grand canonical” implies that the energy-and-particle problem differs significantly from the canonical problem and deserves independent consideration. Analogously, one can redefine the $z$-axis such that the NATS state in Eq. (5) looks identical to the grand canonical ensemble. But this redefinition cannot reduce NATS thermalization to grand canonical, just as a definition cannot reduce grand canonical to canonical.

Finally, if the Hamiltonian has only $U(1)$ symmetry, the thermal state is proportional to an exponential that contains a Hamiltonian that has only $U(1)$ symmetry. The NATS contains a Hamiltonian that has a non-Abelian symmetry. The two states have different group-theoretic properties.

### Appendix B  IN EVERY SHORT-RANGE-CORRELATED STATE, EACH TOTAL SPIN COMPONENT HAS A SUBEXTENSIVE STANDARD DEVIATION.

Consider an arbitrary short-range-correlated state of correlation length $\xi$. Let $\langle O \rangle$ denote the expectation value of an observable $O$ in that state. By assumption,

$$\langle \sigma_j^{(\alpha)} \sigma_{j'}^{(\alpha)} \rangle - \langle \sigma_j^{(\alpha)} \rangle \langle \sigma_{j'}^{(\alpha)} \rangle \sim e^{-|j-j'|/\xi}. \quad (B1)$$

We have set the lattice spacing to one. Let us calculate each term in the standard deviation of $\sigma_j^{\text{tot}}$,

$$\sqrt{\langle (\sigma_j^{\text{tot}})^2 \rangle - \langle \sigma_j^{\text{tot}} \rangle^2}. \quad (B2)$$

The first term has the form

$$\langle (\sigma_j^{\text{tot}})^2 \rangle = \left( \sum_{j=1}^{N} \sum_{j=1}^{N} \sigma_j^{(\alpha)} \right)^2 = \left( \sum_{j=1}^{N} \sum_{j=1}^{N} \sigma_j^{(\alpha)} \right)^2 = \sum_{j=1}^{N} \sum_{j'=1}^{N} \langle \sigma_j^{(\alpha)} \sigma_{j'}^{(\alpha)} \rangle. \quad (B3)$$

The first term on the right-hand side of Eq. (B3) simplifies as

$$\sum_{j=1}^{N} \langle \sum_{j'=1}^{N} \sigma_j^{(\alpha)} \sigma_{j'}^{(\alpha)} \rangle = \sum_{j=1}^{N} \langle 1^\otimes 1^\otimes \sigma_j^{(\alpha)} \rangle = N. \quad (B4)$$

The second term on the right-hand side of Eq. (B3) simplifies under assumption (B1):

$$\sum_{j' \neq j} \langle \sigma_j^{(\alpha)} \sigma_{j'}^{(\alpha)} \rangle = \sum_{j' \neq j} \langle \sigma_j^{(\alpha)} \rangle \langle \sigma_{j'}^{(\alpha)} \rangle + \sum_{j' \neq j} e^{-|j-j'|/\xi}. \quad (B5)$$
The second term has significant contributions only from subterms in which \(j'\) lies within \(\xi\) of \(j\). Hence the \(e^{-|j-j'|/\xi} \sim e^{-\xi/\xi} = \text{const}\). A constant number of such subterms exist. Hence the right-hand side of Eq. (B5) can be approximated with

\[
\sum_{j \neq j'} \langle \sigma_{\alpha}^{(j)} \sigma_{\alpha}^{(j')} \rangle \sim \sum_{j \neq k} \langle \sigma_{\alpha}^{(j)} \sigma_{\alpha}^{(j')} \rangle + Nn. \tag{B6}
\]

Substituting from Eqs. (B4) and (B6) into the right-hand side of Eq. (B3) yields

\[
\langle (\sigma_{\alpha}^{\text{tot}})^2 \rangle \sim Nn + \sum_{j \neq j'} \langle \sigma_{\alpha}^{(j)} \rangle \langle \sigma_{\alpha}^{(j')} \rangle. \tag{B7}
\]

Let us estimate the second term in (B2):

\[
\langle \sigma_{\alpha}^{\text{tot}} \rangle^2 = \left( \sum_{j=1}^{N_n} \langle \sigma_{\alpha}^{(j)} \rangle \right)^2 = \left( \sum_{j=1}^{N_n} \langle \sigma_{\alpha}^{(j)} \rangle \right) \left( \sum_{j'=1}^{N_n} \langle \sigma_{\alpha}^{(j')} \rangle \right) = \sum_{j=1}^{N_n} \langle \sigma_{\alpha}^{(j)} \rangle^2 + \sum_{j \neq j'} \langle \sigma_{\alpha}^{(j)} \rangle \langle \sigma_{\alpha}^{(j')} \rangle
\]

\[
\sim Nn + \sum_{j \neq j'} \langle \sigma_{\alpha}^{(j)} \rangle \langle \sigma_{\alpha}^{(j')} \rangle. \tag{B8}
\]

We have approximated the first term with (number of terms)(operator norm of \(\sigma_{\alpha}^{(j)}\)). Let us substitute from Eqs. (B7) and (B10) into Eq. (B2). The \(\sum_{j \neq k}\) terms cancel exactly, leaving

\[
\sqrt{\langle (\sigma_{\alpha}^{\text{tot}})^2 \rangle - \langle \sigma_{\alpha}^{\text{tot}} \rangle^2} \sim \sqrt{Nn}. \tag{B11}
\]

Appendix C  SOFT MEASUREMENT

This appendix details the soft measurements introduced in Sec. [I]. We formalize soft measurements in App. C.1 Appendix C.2 provides physical intuition about the preparation procedure that relies on soft measurements.

C 1 Formalization of soft measurements

We formalize soft measurements with a positive operator-valued measure (POVM). POVMs model generalized measurements in QI theory [52]. A POVM consists of positive operators \(M_{\ell} > 0\), called Kraus operators. They satisfy the completeness relation \(\sum_{\ell} M_{\ell} M_{\ell}^\dagger = 1\). Measuring the \(\{M_{\ell}\}\) of a state \(\rho\) has a probability \(\text{Tr}(M_{\ell}^\dagger M_{\ell} \rho)\) of yielding outcome \(\ell\). The measurement updates \(\rho\) to \(M_{\ell} \rho M_{\ell}^\dagger / \text{Tr}(M_{\ell}^\dagger M_{\ell} \rho)\). Let \(P_{\alpha}^{S_{\alpha}}\) denote the projector onto the eigenvalue-\(S_{\alpha}\) eigenspace of \(\sigma_{\alpha}^{\text{tot}}\). A soft \(\sigma_{\alpha}^{\text{tot}}\) measurement has the form \(\{M_{\alpha}^{S_{\alpha}}\}\). The outcome \(S_{\alpha}\) labels the Kraus operators,

\[
M_{\alpha}^{S_{\alpha}} = \sum_{\tilde{S}_{\alpha} = -N_{n}, -N_{n} + 2, \ldots, N_{n} - 2, N_{n}} \sqrt{f_{Nn}(S_{\alpha}, \tilde{S}_{\alpha})} P_{\alpha}^{\tilde{S}_{\alpha}}. \tag{C1}
\]

Outputting \(S_{\alpha}\), the measurement projects the state a little onto each of the eigenspaces in superposition. How much does the measurement project onto the eigenspace associated with some eigenvalue \(\tilde{S}_{\alpha}\)? The amount depends on the amplitude \(f_{Nn}(S_{\alpha}, \tilde{S}_{\alpha})\). The amplitude must maximize where \(S_{\alpha} = \tilde{S}_{\alpha}\), to satisfy the peaking requirement (Sec. [I]). The binomial distribution suggests itself. We present the distribution, then derive and analyze it:

\[
f_{Nn}(S_{\alpha}, \tilde{S}_{\alpha}) = \left( \frac{N_{n}}{2(N_{n} + S_{\alpha})} \right) \left[ \frac{1}{2} \left( 1 + \frac{\tilde{S}_{\alpha}}{N_{n}} \right) \right]^{\frac{1}{2}(N_{n} + S_{\alpha})} \left[ \frac{1}{2} \left( 1 - \frac{\tilde{S}_{\alpha}}{N_{n}} \right) \right]^{\frac{1}{2}(N_{n} - S_{\alpha})}. \tag{C2}
\]

We define \(0^0 = 0\). Numerics confirm that the POVM (C1) satisfies the mild-disturbance condition (ii) in Sec. [I]
The envelope (C2) is constructed as follows. We semiclassically model each qubit as pointing upward or downward along the α-axis. We formulate the binomial probability that an (Nn)-qubit chain has a magnetization Sα, if the average-over-trials magnetization equals ˜Sα. Let n↑ and n↓ denote the numbers of upward- and downward-pointing qubits in some configuration. Let p↑ denote the probability that a given qubit points upward and p↓, the probability that the qubit points downward. We must solve for each of these quantities in terms of Sα, ˜Sα, and Nn. As Nn = n↑ + n↓ and Sα = n↑ − n↓, n↑ = 1/2(Nn + Sα), and n↓ = 1/2(Nn − Sα). On average, ˜Sα = (p↑ − p↓)Nn qubits point upward. By normalization, p↑ = 1 − p↓. Hence p↑ = 1/2(1 + ˜Sα/Nn), and p↓ = 1/2(1 − ˜Sα/Nn). The binomial function has the form fNn(Sα, ˜Sα) = (Nn/n↑)(p↑)n↑(p↓)n↓. Substituting in yields Eq. (C2).

As Nn → ∞, the binomial approaches a Gaussian. The Gaussian has a mean of ⟨Sα⟩ = ˜Sα and a standard deviation of

$$\Delta = \frac{1}{2} \left( Nn \left( 1 + \frac{\tilde{S}_\alpha}{Nn} \right) \left( 1 - \frac{\tilde{S}_\alpha}{Nn} \right) \right) \sim \sqrt{Nn}. \quad (C3)$$

Hence

$$\lim_{Nn \to \infty} f_{Nn}(S_\alpha, ˜S_\alpha) = \exp \left( -\frac{(S_\alpha - ˜S_\alpha)^2}{2\Delta^2} \right) / \sqrt{2\pi\Delta^2}. \quad (C4)$$

**Prima facie**, Sα and ˜Sα appear to have been swapped relative to their natural roles: Sα was defined as the “expected” σαtot value in Sec. I. But ˜Sα determines the mean spin in Eq. (C2). This swap impacts the function’s behavior little: fNn(Sα, ˜Sα) peaks at Sα = ˜Sα. The peak grows higher and narrower as Nn grows. As Nn → ∞, the envelope approaches a Gaussian symmetric under Sα ↔ ˜Sα [Eq. (C4)]. Normalization motivates the swap: The POVM (C1) must satisfy the completeness condition \( \sum_{S_\alpha} (M_{S_\alpha}^\dagger) M_{S_\alpha} = 1 \). The POVM does because the envelope is normalized as \( \sum_{S_\alpha} f_{Nn}(S_\alpha, ˜S_\alpha) = 1 \).

### C 2 Physical intuition about the soft-measurement preparation procedure

Suppose that the spin chain begins in a random state. Measuring \( H^{\text{tot}} \) with decent precision projects the chain’s state approximately onto an energy eigenspace. This eigenspace is larger than the a.m.c. subspace, \( \mathcal{M} \). The soft \( x \) measurement collapses the state a little, shrinking the state’s support. The soft \( y \) and \( z \) measurements shrink the support further. After the final measurement, at least most of the state’s support lies in \( \mathcal{M} \), as quantified in App. I. Figure 3 sketches the relationships amongst the subspaces.

**FIG. 3: Sketch of subspaces**: The black, outermost line represents an eigenspace of the total Hamiltonian, \( H^{\text{tot}} \). Inside lies the approximate microcanonical subspace, \( \mathcal{M} \), represented by the shaded shape. \( \mathcal{M} \) generalizes the microcanonical subspace to noncommuting exchanged charges. The total-spin components \( \sigma_{a=x,y,z}^{\text{tot}} \) have eigenspaces that largely coincide with \( \mathcal{M} \).

Let us illustrate how each soft measurement partially collapses the spin chain’s state. Consider a toy system of Nn = 2 qubits whose \( \sigma_z^{\text{tot}} \) and \( \sigma_x^{\text{tot}} \) are measured softly. Suppose that the measurements yield \( S_z, S_x = 0 \). The conditioned soft \( z \) measurement projects the state with \( P_z^0 \propto M_z^0 \), by Eqs. (C1) and (C2). \( P_z^0 \) projects onto the eigenvalue-0 eigenspace of \( \sigma_z^{\text{tot}} \). This eigenspace is spanned by the singlet \( |s_z\rangle := \frac{1}{\sqrt{2}} (|z+, z-\rangle - |z-, z+\rangle) \) and the
entangled triplet $|t_z\rangle := \frac{1}{\sqrt{2}} (|z+,z-\rangle + |z-,z+\rangle)$. That is, $P^0_x = |s_z\rangle\langle s_z| + |t_z\rangle\langle t_z|$. Similarly, the conditioned $x$ measurement projects the state with $P^0_x = |s_x\rangle\langle s_x| + |t_x\rangle\langle t_x|$.

Onto what subspace does the sequence of approximate measurements project? Let us express $P^0_x$ in terms of the $z$-type singlet and triplets. The singlet relative to any axis equals the singlet relative to every other, to within a global phase: $|s_x\rangle = \langle \text{phase} |s_z\rangle$. The $x$-type entangled triplet decomposes as $|t_x\rangle \propto \frac{1}{\sqrt{2}} (|z+,z+\rangle - |z-,z-\rangle)$. Hence $P^0_x P^0_x = |s_x\rangle\langle s_x|$. The approximate $\sigma^{\text{tot}}_z$ measurement collapses the state onto a two-dimensional subspace; and the approximate $\sigma^{\text{tot}}_x$ measurement, onto a one-dimensional subspace.

### Appendix D  PARAMETERIZATION OF THE APPROXIMATE MICROCANONICAL SUBSPACE

An a.m.c. subspace $\mathcal{M}$ is defined in terms of five small parameters [7]. They govern the constants in Ineq. (16), the bound on the distance between $\rho_S$ and the NATS. The constants’ forms are calculated partially in [7]. Calculating them completely would require experiments or extensive analytics. We review the a.m.c. subspace’s definition in Sec. D 1. In Sec. D 2, we identify parameter values suited to our protocol.

#### D 1 Definition of the a.m.c. subspace

$\mathcal{M}$ is defined in terms of two conditions [7]: (i) Every state in $\mathcal{M}$ has a fairly well-defined value of each $\sigma^{\text{tot}}_\alpha$. (ii) Consider state whose $\sigma^{\text{tot}}_\alpha$ has a fairly well-defined value for every $\alpha$. Most of the state’s support lies in $\mathcal{M}$. These conditions are quantified in terms of small parameters $\delta, \eta, \delta', \eta', \epsilon \geq 0$.

(i) Let $\omega$ denote any whole-system state supported in just $\mathcal{M}$. In $\omega$, every total charge has a fairly well-defined value: Consider measuring any $\sigma^{\text{tot}}_\alpha$. The measurement has a high probability of yielding an outcome close to the “expected value” $S_\alpha$. (The notation $v_\alpha = S_\alpha$ is used in [7].) Consider a narrow strip of $\sigma^{\text{tot}}_\alpha$ eigenvalues centered on $S_\alpha$. Recall that the system-of-interest charge $\sigma^{j}_\alpha + \sigma^{j+1}_\alpha$ has a spectral diameter of two. The strip is therefore chosen to extend a distance $2\eta N$ on either side of $S_\alpha$. Consider the $\sigma^{\text{tot}}_\alpha$ eigenvalues in $[S_\alpha - 2\eta N, S_\alpha + 2\eta N]$. They correspond to eigenspaces whose direct sum is projected onto by $\Pi_\alpha^0$. A $\sigma^{\text{tot}}_\alpha$ measurement has a probability $\text{Tr}(\omega \Pi^0_\alpha)$ of yielding a value in this interval. The probability must be at least $1 - \delta$:

$$\text{supp}(\omega) \subset \mathcal{M} \Rightarrow \text{Tr}(\omega \Pi^0_\alpha) \geq 1 - \delta \quad \forall \alpha.$$  \tag{D1}

(ii) Let $\omega'$ denote any state for which measuring any $\sigma^{\text{tot}}_\alpha$ has a high probability of yielding an outcome close to the expected value, within $2\eta' N$ of $S_\alpha$. Most of the support of $\omega'$ lies in $\mathcal{M}$—at least a fraction $1 - \epsilon$. As $F_\mathcal{M}$ denotes the projector onto the a.m.c. subspace,

$$\text{Tr}(\omega' \Pi^0_\alpha) \geq 1 - \delta' \quad \forall \alpha \quad \Rightarrow \quad \text{Tr}(\omega' P_\mathcal{M}) \geq 1 - \epsilon.$$  \tag{D2}

#### D 2 Parameter values suited to the soft-measurement preparation procedure

We focus on the soft-measurement state preparation for concreteness. After the procedure, measuring any $\sigma^{\text{tot}}_\alpha$ likely yields a value within a standard deviation $\Delta$ of $S_\alpha$. The standard deviation scales as $\Delta \sim \sqrt{N\eta}$. Hence the procedure prepares an instance of the $\omega'$ in [D2], for $2\eta' N = (\text{const.}) \sqrt{N\eta}$. Rearranging yields the first small parameter,

$$\eta' = (\text{const.})/\sqrt{N}.$$  \tag{D3}

We have incorporated $\sqrt{N} = \sqrt{2}$ into the constant. The spin chain is large, so $\eta'$ is small, as desired.

We choose $\delta'$ by calculating the left-hand side of the leftmost inequality in [D2], the probability that measuring a $\sigma^{\text{tot}}_\alpha$ of $\omega'$ yields a value within $\Delta$ of $S_\alpha$. We integrate $f_{N_\eta}(S_\alpha, \tilde{S}_\alpha)$ across a region, centered on $\tilde{S}_\alpha = S_\alpha$, of half-width $\Delta$:

$$1 - \delta' \leq \int_{S_\alpha - \Delta}^{S_\alpha + \Delta} d\tilde{S}_\alpha f_{N_\eta}(S_\alpha, \tilde{S}_\alpha).$$  \tag{D4}
We approximate \( f_{\text{Nn}} \) with the Gaussian \( \text{(C4)} \). A Gaussian is well-known to have 68% of its weight within a standard deviation of its mean. Hence we choose \( 1 - \delta' = 0.68 \), or
\[
\delta' = 0.32. \tag{D5}
\]
\( \delta' \) is close to zero, as desired.

We have chosen values for two of the five parameters that define an a.m.c. subspace \( \mathcal{M} \), \( \eta' \) and \( \delta' \). Let us turn to \( \eta, \delta, \) and \( \epsilon \). In \( \text{[2]} \), \( c \) denotes the number of non-Hamiltonian charges. Theorem 4 in \( \text{[7] Suppl. Inf.} \) presents a condition under which \( \mathcal{M} \) is known to exist. The condition governs the small parameters and the number \( N \) of subsystems:

For every \( \epsilon > (c+1)\delta' > 0, \eta > \eta' > 0, \delta > 0, \) and all great-enough \( N \), “there exists an \((\epsilon, \eta, \eta', \delta, \delta')\)-approximate microcanonical subspace \( \mathcal{M} \) [. . .] associated with [. . .] the approximate expectation values” \( S_\alpha \). An \( \mathcal{M} \) might exist under other conditions. But these known conditions motivate choices of \( \epsilon \) and \( \eta \). The theorem suggests choosing
\[
\eta > \eta' = \text{(const.)} / \sqrt{N}. \tag{D6}
\]
By Eq. \( \text{(D4)} \) and \( c = 3 \),
\[
\epsilon > (c+1)\delta' = 1.28. \tag{D7}
\]
Though \( \epsilon > 1 \) contradicts the spirit of the a.m.c. subspace’s definition, the inequality does not contradict the letter.

We have chosen values for all the parameters except \( \delta \). Our preparation procedure, even supplemented with Theorem 4 of \( \text{[7] Suppl. Inf.} \), underdetermines \( \delta \). However, viewing the \( \omega \) in Eq. \( \text{(D1)} \) loosely as the \( \omega' \) in Eq. \( \text{(D2)} \) can be informative. We therefore choose
\[
\delta = \delta' = 0.32. \tag{D8}
\]

Appendix E  CALCULATION OF THE INVERSE TEMPERATURE \( \beta \) AND THE EFFECTIVE CHEMICAL POTENTIALS \( \mu_\alpha \)

Let us derive Eqs. \( \text{(13)} \) and \( \text{(14)} \). We index such that \( S \) consists of qubits \( j = 1, 2, \ldots, n \). This choice is for convenience, and \( S \) lies far from the boundaries. We assume that the temperature is high and the chemical potentials are low: Calculations are to first order in the small parameters approximated in the left-hand side of Ineq. \( \text{(12)} \) and presented precisely below [in Ineq. \( \text{(E14)} \) for closed boundary conditions and in Ineq. \( \text{(E16)} \) for periodic]. We calculate the partition function, then \( \beta \), and then the \( \mu_\alpha \)’s. Rewriting Eq. \( \text{(10)} \) will prove convenient:
\[
H_{\text{tot}} = J \sum_{\alpha=x,y,z} \left( \sum_{j=1}^{N-n-1} \sigma_\alpha^{(j)} \sigma_\alpha^{(j+1)} + \sum_{j=1}^{N-n-2} \sigma_\alpha^{(j)} \sigma_\alpha^{(j+2)} \right). \tag{E1}
\]
This Hamiltonian encodes closed boundary conditions. The numerical simulations (Sec. \( \text{[II]} \)) involve periodic boundary conditions. We extend calculations to periodic boundary conditions at the end of the appendix.

**Partition function:** Let us Taylor-approximate the exponential in the NATS:
\[
e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha \sigma_\alpha^{\text{tot}})} = 1 - \beta H_{\text{tot}} + \beta^2 \sum_\alpha \mu_\alpha \sigma_\alpha^{\text{tot}} + O_2. \tag{E2}
\]
The exponential’s trace equals \( Z \). The linear terms vanish, as Tr(\( \sigma_\alpha^{(j)} \)) = 0 for all \( \alpha \) and \( j \). Hence
\[
Z = 2^{Nn} + O_2. \tag{E3}
\]

**Inverse temperature:** \( \beta \) follows from the prediction
\[
E_{\text{tot}} = \frac{\text{Tr} \left( H_{\text{tot}} e^{-\beta (H_{\text{tot}} - \sum_\alpha \mu_\alpha \sigma_\alpha^{\text{tot}})} \right)}{Z}. \tag{E4}
\]
We substitute in for the exponential from Eq. \( \text{(E2)} \), then invoke the trace’s linearity. Terms one and three vanish by the Paulis’ tracelessness:
\[
E_{\text{tot}} = -\beta \text{Tr} \left( \left[ H_{\text{tot}} \right]^2 \right) / Z + O_2. \tag{E5}\]
Let us evaluate the trace:

\[
\text{Tr} \left( \left[ H^{\text{tot}} \right]^2 \right) = J^2 \sum_{\alpha, \alpha'} \text{Tr} \left( \sum_{j, j'=1}^{Nn-1} \sigma_{\alpha}^{(j)} \sigma_{\alpha'}^{(j+1)} \sigma_{\alpha'}^{(j')} \sigma_{\alpha}^{(j'+1)} + \sum_{j=1}^{Nn-2} \sum_{j'=1}^{Nn-1} \sigma_{\alpha}^{(j)} \sigma_{\alpha'}^{(j+1)} \sigma_{\alpha'}^{(j')} \sigma_{\alpha}^{(j'+2)} + \sum_{j=1}^{Nn-2} \sum_{j'=1}^{Nn-1} \sigma_{\alpha}^{(j)} \sigma_{\alpha'}^{(j+2)} \sigma_{\alpha'}^{(j')} \sigma_{\alpha}^{(j'+2)} \right). 
\]

Most of the terms vanish, by the Paulis’ tracelessness. In each surviving term, \( \alpha = \alpha', j = j' \), and the second Pauli operator acts on the same qubit as the fourth. Every Pauli squares to the identity, \( \left( \sigma_{\alpha}^{(j)} \right)^2 = 1 \), so

\[
\text{Tr} \left( \left[ H^{\text{tot}} \right]^2 \right) = J^2 \sum_{\alpha} \left( \sum_{j=1}^{Nn-1} + \sum_{j=1}^{Nn-2} \right) 2^{Nn} = 3(2Nn-3)2^{Nn}J^2. 
\]

We substitute into Eq. (E5):

\[
E^{\text{tot}} = -3(2Nn-3)\beta J^2 + O_2. \tag{E9}
\]

Solving for \( \beta \) yields Eq. (13).

**Effective chemical potentials:** \( \mu_\alpha \) follows from the prediction

\[
S_\alpha = \text{Tr} \left( \sigma_{\alpha}^{\text{tot}} e^{-\beta \left( H^{\text{tot}} - \sum_{\alpha'} \mu_{\alpha'} \sigma_{\alpha'}^{\text{tot}} \right)} \right) / Z. \tag{E10}
\]

We Taylor-approximate the exponential as in Eq. (E2), then invoke the trace’s linearity. Terms one and two vanish, by the Paulis’ tracelessness:

\[
S_\alpha = \left[ \beta \sum_{\alpha'} \mu_{\alpha'} \text{Tr} \left( \sigma_{\alpha}^{\text{tot}} \sigma_{\alpha'}^{\text{tot}} \right) + O_2 \right] / Z. \tag{E11}
\]

The trace evaluates to

\[
\text{Tr} \left( \sigma_{\alpha}^{\text{tot}} \sigma_{\alpha'}^{\text{tot}} \right) = \sum_{j, j'=1}^{Nn} \text{Tr} \left( \sigma_{\alpha}^{(j)} \sigma_{\alpha'}^{(j')} \right) = Nn 2^{Nn} \delta_{\alpha \alpha'}. \tag{E12}
\]

In the sum’s nonzero terms, the two Pauli operators collide. We substitute into Eq. (E11) and solve for \( \mu_\alpha \):

\[
\mu_\alpha = \frac{S_\alpha}{Nn\beta} + O_2. \tag{E13}
\]

Substituting in for \( \beta \) from Eq. (13) yields Eq. (14).

**Small-parameter conditions:** Inequalities (12) specify loosely when our Taylor approximations hold. More-precise forms for the conditions are presented here. The conditions follow from calculating second-order corrections, then demanding that the corrections be much smaller than the first-order terms:

\[
\sqrt{3(2Nn-3)} |\beta|J, \sqrt{Nn} \sum_\alpha \mu_\alpha^2 |\beta|, \frac{2}{3} \beta \sum_\alpha \mu_\alpha^2 J, 6 \frac{Nn-2}{2Nn-3} |\beta|J, 4 \frac{2Nn-3}{Nn} |\beta|J \ll 1. \tag{E14}
\]

**Periodic boundary conditions:** The numerical simulations (Sec. 11) involve periodic boundary conditions. The Hamiltonian has the form

\[
H^{\text{tot}} = J \sum_{\alpha} \sum_{j=1}^{Nn} \left( \sigma_{\alpha}^{(j)} \sigma_{\alpha}^{(j+1)} + \sigma_{\alpha}^{(j)} \sigma_{\alpha}^{(j+2)} \right). \tag{E15}
\]

The site label \( j = Nn + 1 \) is defined as \( j = 1 \), and \( j = Nn + 2 \) is defined as \( j = 2 \). Equation (E8) changes to

\[
\text{Tr} \left( \left[ H^{\text{tot}} \right]^2 \right) = 6Nn 2^{Nn} J^2, \text{ so } \beta = -\frac{2 \mu_{\text{tot}}}{6Nn J^2} + O_2. \tag{E18}
\]

The \( \mu_\alpha \) prediction remains unchanged to first order, though not to second-order. The small-parameter conditions become

\[
\sqrt{6Nn} |\beta|J, \frac{2}{3} |\beta| \sum_\alpha \mu_\alpha^2 J, 8 |\beta|J \ll 1. \tag{E16}
\]
Appendix F  QUANTUM STATE TOMOGRAPHY FOR INFERRING THE LONG-TIME SYSTEM-OF-INTEREST STATE

We aim to observe that $S$, the $n$-qubit system of interest, thermalizes to the NATS. The following quantum-state-tomography protocol suffices. A more efficient protocol, that takes advantage of the NATS’s form, might exist.

Let $\vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ specify a product $\sigma_{m_1}^{(1)} \otimes \sigma_{m_2}^{(2)} \otimes \ldots \otimes \sigma_{m_n}^{(n)}$ of Pauli operators. $3^n$ such products exist. The set of the products’ eigenbases forms a basis for the $n$-qubit Hilbert space. We measure each eigenbasis at the end of each of $N_{\text{trials}}$ trials. Each measurement yields one of $2^n$ possible outcomes, $\ell = 1, 2, \ldots, 2^n$. If outcome $\ell$ obtains, the projector $\Pi_\ell^\alpha$ projects the state. Each measurement has a probability $p(\ell | \rho_S) = \text{Tr}(\Pi_\ell^\alpha \rho_S)$ of yielding outcome $\ell$. Let $f_\ell^\alpha$ denote the frequency with which measuring $\vec{\alpha}$ yields outcome $\ell$ in our $N_{\text{trials}}$ trials. The frequency approximates the probability with an error $\sim 1/\sqrt{N_{\text{trials}}}$.

From the frequencies, we estimate $\rho_S$. We can do so by solving the semidefinite program

$$\min_{\rho \geq 0, \text{Tr}(\rho) = 1} \sum_{\vec{a} \in \{x,y,z\}^n} \sum_{\ell=0}^{2^n-1} \left[ f_\ell^\vec{a} - \text{Tr}(\Pi_\ell^\vec{a} \rho) \right]^2.$$  \hfill (F1)

Solving this program is equivalent, in the limit of large $N_{\text{trials}}$ and so Gaussian noise, to maximizing the likelihood function that generated the frequencies.

We can solve the program (F1) efficiently by recasting the frequencies in terms of expectation values. Knowing $2^n$ probabilities, we can calculate the expectation values of $2^n - 1$ products of Pauli operators and identity operators. $4^n - 1$ such products exist. They have the form $\sigma_{m_1}^{(1)} \otimes \sigma_{m_2}^{(2)} \otimes \ldots \otimes \sigma_{m_n}^{(n)}$. The $j^\text{th}$ qubit’s $m_j = 0, x, y, z$; and $\sigma^{(j)}_{m_j} = 1(j)$. Consider, for example, a system of $n = 2$ qubits. Suppose that we know the four probabilities $p(x,z)\; p(x,-z)\; p(-x,z)\; p(-x,-z)$. We can calculate three expectation values, $\langle \sigma_x \otimes \sigma_z \rangle$, $\langle \sigma_x \otimes 1 \rangle$, and $\langle 1 \otimes \sigma_z \rangle$. Hence solving the program (F1) is equivalent to solving

$$\min_{\rho \geq 0, \text{Tr}(\rho) = 1} \sum_{m \in \{0,x,y,z\}^n} \left\{ \left\langle \sigma_{m_1}^{(1)} \otimes \ldots \otimes \sigma_{m_n}^{(n)} \right\rangle - \text{Tr} \left( [\sigma_{m_1}^{(1)} \otimes \ldots \otimes \sigma_{m_n}^{(n)}] \rho \right) \right\}^2.$$  \hfill (G1)

The expectation values $\left\langle \sigma_{m_1}^{(1)} \otimes \ldots \otimes \sigma_{m_n}^{(n)} \right\rangle$ are calculated from the measurement data.

The program (G2) can be solved efficiently as follows [62]. First, we solve the linear inversion problem

$$\min_{\rho \geq 0} \sum_{m \in \{0,x,y,z\}^n} \left\{ \left\langle \sigma_{m_1}^{(1)} \otimes \ldots \otimes \sigma_{m_n}^{(n)} \right\rangle - \text{Tr} \left( [\sigma_{m_1}^{(1)} \otimes \ldots \otimes \sigma_{m_n}^{(n)}] \rho \right) \right\}^2.$$  \hfill (G3)

Then, we impose the positive-semidefinite and trace constraints.

Appendix G  PROTOCOL’S ROBUSTNESS WITH RESPECT TO EXPERIMENTAL ERROR

In [44], a nearly isotropic Heisenberg model is effected with a Bose-Hubbard Hamiltonian in the hardcore limit. The Hamiltonian has the form

$$H_{BH} = -J_{ex} \sum_j \left[ 2 \left( \sigma_{x}^{(j)} \sigma_{x}^{(j+1)} + \sigma_{-x}^{(j)} \sigma_{-x}^{(j+1)} \right) + \Delta \sigma_{z}^{(j)} \sigma_{z}^{(j+1)} \right].$$  \hfill (G1)

Again, we have ignored factors of $\hbar/2$. $J_{ex}$ denotes the energy scale, and $\Delta$ denotes the isotropy parameter. $H_{BH}$ becomes an isotropic Heisenberg model when $\Delta = 1$. When $\Delta \neq 1$, angular momenta associated with different axes hop at different rates. $H_{BH}$ consequently conserves only $\sigma_z$ and $\sigma_y$. An isotropy parameter of $\Delta = 0.986$ was achieved in the experiment.

We investigated our protocol’s robustness with respect to this error. We simulated evolution under a Hamiltonian that resembles (G1) but that encodes next-nearest-neighbor couplings:

$$\tilde{H}_{BH} = -J_{ex} \sum_{j=1}^{N_n} \left( \sigma_{x}^{(j)} \sigma_{x}^{(j+1)} + \sigma_{y}^{(j)} \sigma_{y}^{(j+1)} + \Delta \sigma_{z}^{(j)} \sigma_{z}^{(j+1)} \right) + \sum_{j=1}^{N_n} \left( \sigma_{x}^{(j)} \sigma_{x}^{(j+2)} + \sigma_{y}^{(j)} \sigma_{y}^{(j+2)} + \Delta \sigma_{z}^{(j)} \sigma_{z}^{(j+2)} \right).$$  \hfill (G2)
As in Sec. II, we simulated periodic boundary conditions. We chose for the nearest-neighbor and next-nearest-neighbor terms to have the same $\Delta$. We focused on a 1% anisotropy and set $J_{ex} = 1$. To mitigate the error, we implemented the scheme in [47] (Sec. I): The evolution time $t = 2Nn$ was split into steps of duration $dt = t/(3 \times 2Nn + 1)$. After each time step, the system underwent a 90° rotation. (Qubits can be rotated experimentally with microwave pulses.) The $x$-axis was rotated into the $y$-axis, then into the old $z$-axis, and then returned to its original orientation. This cycle was then repeated.

Figure 4 shows the resulting relative entropies. Each state was calculated from $H^{tot}$, as though the error were absent. For example, $\rho_{\text{NATS}}$ continues to have the form in Eq. (2). The NATS prediction remains the most accurate, despite the simulated experimental error.

**FIG. 4:** Protocol’s robustness with respect to anisotropy: Experimental implementations of the Heisenberg Hamiltonian [10] may involve anisotropic couplings. Evolution under the Hamiltonian [12] was simulated with an isotropy parameter of $\Delta = 0.99$, in mimicry of the experiment in [44].

REFERENCES