# Estimation of Hamiltonian parameters from thermal states 

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#### Abstract

We upper- and lower-bound the optimal precision with which one can estimate an unknown Hamiltonian parameter via measurements of Gibbs thermal states with a known temperature. The bounds depend on the uncertainty in the Hamiltonian term that contains the parameter and on the term's degree of noncommutativity with the full Hamiltonian: higher uncertainty and commuting operators lead to better precision. We apply the bounds to show that there exist entangled thermal states such that the parameter can be estimated with an error that decreases faster than $1 / \sqrt{n}$, beating the standard quantum limit. This result governs Hamiltonians where an unknown scalar parameter (e.g. a component of a magnetic field) is coupled locally and identically to $n$ qubit sensors. In the high-temperature regime, our bounds allow for pinpointing the optimal estimation error, up to a constant prefactor. Our bounds generalize to joint estimations of multiple parameters. In this setting, we recover the high-temperature sample scaling derived previously via techniques based on quantum state discrimination and coding theory. In an application, we show that noncommuting conserved quantities hinder the estimation of chemical potentials.


Substantial work has been devoted to determining the precision with which a Hamiltonian parameter can be estimated from measurements on a time-evolving system. For instance, consider a spin network immersed in a magnetic field $\mu$. The network's state acquires information about the field's magnitude. Measuring copies of the state can reveal $\mu$. The quantum Cramér-Rao bound sets an asymptotically saturable lower bound on the precision with which the parameter can be estimated [1, 2].

Here, we focus on the less explored problem of estimating parameters from systems in a thermal state

$$
\begin{equation*}
\rho=\frac{1}{Z_{\beta}} e^{-\beta H}=\frac{1}{Z_{\beta}} \sum_{j} e^{-\beta \omega_{j}}|j\rangle\langle j| \tag{1}
\end{equation*}
$$

at a known inverse temperature $\beta$. $\omega_{j}$ and $|j\rangle$ are the Hamiltonian's eigenvalues and eigenvectors, $H=\sum_{j} \omega_{j}|j\rangle\langle j|$, and $Z_{\beta}:=\operatorname{Tr}\left(e^{-\beta H}\right)$ is the partition function. Parameters of $H$ could be unknown. The system could thermalize to $\rho$ through interactions with a thermal environment or through a state-preparation algorithm [3, 4]. Probing the environment could yield information about $\beta$ [5].

The thermal state encodes information about the Hamiltonian parameters. We consider $M$-term Hamiltonians:

$$
\begin{equation*}
H=\sum_{l=1}^{M} H_{l}=\sum_{l=1}^{M} \mu_{l} A_{l} \tag{2}
\end{equation*}
$$

[^0]The $A_{l}$ are Hermitian operators, and the $\mu_{l}$ are real coefficients. The $\mu_{l}$ could represent local or global fields or coupling constants (Fig. 1). We bound the precision with which the $\mu_{l}$ can be estimated from measurements of copies of $\rho$. To achieve this goal, we will use the multiparameter quantum Cramér-Rao bound, which constrains the estimation of a set of parameters [6].

The quantum Cramér-Rao bound relates the minimum estimation error to the quantum Fisher information [7]. The quantum Cramér-Rao bound has been applied, for example, to the field of thermometry [5, 8-13]. The bound implies the minimum uncertainty with which a temperature $T$ can be estimated from $\mathcal{N}$ measurements: $\operatorname{var}\left(\hat{T}_{\text {opt }}\right)=T^{4} \frac{1}{\mathcal{N}(\Delta H)^{2}}$, where $(\Delta H)^{2}:=\left\langle H^{2}\right\rangle-\langle H\rangle^{2}$ is the Hamiltonian's variance in the thermal state [6]. Whenever $x$ denotes a parameter to be estimated, we mean by $\hat{x}$ an estimator. Higher energy variances allow for better parameter estimation. This result echoes the relative error $\operatorname{var}\left(\hat{\mu}_{\mathrm{opt}}\right) / \mu^{2}=\frac{1}{4 \mathcal{N} t^{2}(\Delta H)^{2}}$ with which a global parameter $\mu$ can be estimated from measurements of copies of a pure state evolving under the Hamiltonian $H=\mu A$ for a time $t$. In related work, Refs. [14, 15] geometrically characterize the Fisher metric to study the role of phase transitions in thermometry. This Letter focuses on the error in estimates of an arbitrary Hamiltonian parameter, rather than the error in temperature estimation.

Several studies have concerned the reconstruction of a Hamiltonian from its eigenstates [16-22], from steady states [23], or from Gibbs states [22, 24]. Recent results under the umbrella of the "Hamiltonian-learning problem" provide algorithms for estimating Hamiltonian pa-


FIG. 1. Estimating Hamiltonian parameters from thermal states. How accurately can one determine $\mu_{l}$, which can be a coupling constant-pictured here as yellow and teal dashed lines for a system of qubits on a lattice - or a field, in a Hamiltonian $H$ from measurements performed on $\mathcal{N}$ copies of a thermal state $\rho=e^{-\beta H} / Z_{\beta}$ ? We use the quantum Cramér-Rao bound to derive saturable upper and lower bounds on the optimal precision with which such Hamiltonian parameters can be estimated.
rameters while minimizing (i) the number of copies of the thermal state $\rho$ needed (the sample complexity) and (ii) the algorithm's runtime (the time complexity) [25-28]. Such complexity-theoretic approaches focus on (a) the asymptotic sample and time complexities' dependence on $\beta$ and (b) the number of unknown parameters. In contrast, we leverage the quantum Cramér-Rao bound to identify how the uncertainties in the $A_{l} \mathrm{~s}$, and the $A_{l} \mathrm{~s}$ ' noncommutativity with the thermal state, influence the minimum precision with which the $\mu_{l}$ can be estimated. Upon pinpointing the uncertainties' influence on precision, we can construct a many-body model that beats the standard quantum limit.

This Letter is organized as follows. First, we review the quantum Fisher information, a powerful tool for analyzing parameter estimation. We bound the quantum Fisher information obtainable about one Hamiltonian parameter, then bound the precision with which the parameter can be estimated. These bounds enable us to identify a many-body model in which the achievable precision beats the standard quantum limit. Extending beyond one Hamiltonian parameter, we then bound the precision with which multiple parameters can be estimated simultaneously. Finally, we discover that noncommutation of conserved quantities (charges) hinders the estimation of chemical potentials. Noncommuting charges are particularly quantum (due to the importance of noncommutation in quantum measurement disturbance, Heisenberg uncertainty, etc.) and have been of recent thermodynamic interest [29].

The quantum Fisher information matrix. -The multiparameter quantum Cramér-Rao bound constrains the
statistics of any estimator $\hat{\vec{\mu}}$ of the parameters $\mu_{l}[6]$ :

$$
\begin{equation*}
\operatorname{cov}(\hat{\vec{\mu}}) \geq \frac{1}{\mathcal{N}} \mathcal{F}^{-1} \tag{3}
\end{equation*}
$$

$\mathcal{N}$ denotes the number of experimental repetitions. $\mathcal{F}$ denotes the quantum Fisher information matrix, with components

$$
\begin{equation*}
\mathcal{F}_{l m}:=2 \sum_{j k} \frac{\operatorname{Re}\left[\langle j| \partial_{l} \rho|k\rangle\langle k| \partial_{m} \rho|j\rangle\right]}{p_{j}+p_{k}} \tag{4}
\end{equation*}
$$

The state eigendecomposes as $\rho=\sum_{j} p_{j}|j\rangle\langle j|$. Thus, the quantum Fisher information matrix characterizes the precision with which parameters $\mu_{l}$ can be estimated jointly. The multiparameter quantum CramérRao bound is saturated when the optimal measurements for estimating the $\mu_{l}$ are compatible. Mathematically, this condition is met if and only if $\operatorname{Tr}\left(\rho\left[L_{l}, L_{m}\right]\right)=0$. The symmetric logarithmic derivative $L_{l}$ is implicitly defined by $\partial_{l} \rho=: \frac{1}{2}\left\{\rho, L_{l}\right\}$ [6]. Throughout this work, we denote partial derivatives by $\partial_{l}:=\frac{\partial}{\partial \mu_{l}}$.

The diagonal matrix element $\mathcal{F}_{l l}$ quantifies the minimum precision with which one unknown $\mu_{l}$ can be estimated if all other parameters are known. The singleparameter quantum Cramér-Rao bound says that every estimator $\hat{\mu_{l}}$ has a variance

$$
\begin{equation*}
\operatorname{var}\left(\hat{\mu}_{l}\right) \geq \frac{1}{\mathcal{N} \mathcal{F}_{l l}} \tag{5}
\end{equation*}
$$

Optimized measurements saturate this bound [2, 7]. Equations (3) and (5) thus pinpoint the quantum Fisher information as a powerful tool that determines ultimate limits on quantum metrology. The stronger $\rho$ 's dependency on $\mu_{l}$, the higher the quantum Fisher information $\mathcal{F}_{l l}$ [Eq. (4)], and so the greater the precision.

Bounds on the quantum Fisher information. - Exactly evaluating the quantum Fisher information can be difficult. Therefore, it is desirable to bound $\mathcal{F}_{l l}$ in terms of more-easily-calculable quantities. We derive two sets of upper and lower bounds on the quantum Fisher information of the $\mu_{l}$ in Eq. (2):

$$
\begin{align*}
& \mathcal{F}_{l l} \leq \beta^{2}\left(\Delta A_{l}\right)^{2}  \tag{6a}\\
& \mathcal{F}_{l l} \geq 4 \beta^{2} c_{1}\left(\Delta A_{l}\right)^{2} \tag{6b}
\end{align*}
$$

and

$$
\begin{align*}
\mathcal{F}_{l l} & \leq 2.4 c_{2} \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right) \quad \text { and }  \tag{7a}\\
\mathcal{F}_{l l} & \geq 0.8 \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right) \tag{7b}
\end{align*}
$$

$\Delta A_{l}=\sqrt{\left\langle A_{l}^{2}\right\rangle-\left\langle A_{l}\right\rangle^{2}}$ is the uncertainty of operator $A_{l}$ in $\rho ;\|A\|_{2}^{2}:=\operatorname{Tr}\left(A A^{\dagger}\right)$; and we have defined

$$
\begin{align*}
& c_{1}:=\tanh ^{2}\left(\beta\|H\|_{\mathrm{s}} / 2\right) /\left(\beta\|H\|_{\mathrm{s}}\right)^{2} \quad \text { and }  \tag{8a}\\
& c_{2}:=2 c_{1} \cosh \left(\beta\|H\|_{\mathrm{s}} / 2\right) \tag{8b}
\end{align*}
$$

The $\|H\|_{\mathrm{s}}:=\max _{j} \omega_{j}-\min _{j} \omega_{j}$ is the Hamiltonian seminorm defined by the maximum energy gap. We derive the bounds by computing the thermal state's quantum Fisher information, then algebraically manipulating the expression (Appendix II).

Equation (6) constrains the quantum Fisher information about $\mu_{l}$ in terms of $\Delta A_{l}$, resembling expressions for the quantum Fisher information about $\beta$ in thermometry [6]. Equation (7) constrains the quantum Fisher information about $\mu_{l}$ also in terms of the Wigner-Yanase skew information $\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}$. The skew information was proposed as a means to discriminate quantum and classical contributions to uncertainty [30, 31]. It has found applications in parameter estimation [10, 32, 33], as an asymmetry measure [34], and as a coherence measure $[35,36]$. The difference $\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}$ signifies the classical uncertainty about $A_{l}$ [31]. This classical uncertainty vanishes for pure states.

When the temperature is high relative to the maximum energy gap $\left(\beta\|H\|_{\mathrm{s}} \ll 1\right), c_{1} \approx c_{2} / 2 \approx 1 / 4$. The upper and lower bounds in Eq. (6) coincide, while the upper and lower bounds in Eq. (7) differ by a prefactor of 1.2. That is, our bounds are saturated, up to a constant prefactor, at high temperatures. Our bounds pinpoint $\mathcal{F}_{l l}$ by tightly sandwiching it.

The upper bound (7a) is also saturable, up to a constant prefactor, at low temperatures. To show this, we denote by $\mu$ the magnitude of a field $\mu \sigma_{z}$ acting on a qubit with a Hamiltonian $H=\Omega_{x} \sigma_{x}+\Omega_{z} \sigma_{z}+\mu \sigma_{z}$. The $\sigma_{\alpha}$ S are Pauli matrices. The quantum Fisher information and its upper bound (7a) can be calculated exactly. At low temperatures $\left(\beta\|H\|_{s} \gg 1\right)$, $\mathcal{F}_{\mu} \approx 16 \Omega_{x}^{2} /\|H\|_{s}^{4} \leq 2.4 c_{2} \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right) \approx$ $19.2 \Omega_{x}^{2} /\|H\|_{s}^{4}$; and, at high temperatures $\left(\beta\|H\|_{s} \ll 1\right)$, $\mathcal{F}_{\mu} \approx \beta^{2} \leq 2.4 c_{2} \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right) \approx 1.2 \beta^{2}$ (Appendix IV). The contribution of the Wigner-Yanase skew information is necessary for obtaining a saturable bound at low temperatures.

Reference [10] contains the closest previous result: $\mathcal{F}_{l l} \leq \beta^{2} \int_{0}^{1} \operatorname{Tr}\left(\rho^{a} \delta A_{l} \rho^{1-a} \delta A_{l}\right) d a$, with $\delta A_{l}:=A_{l}-\left\langle A_{l}\right\rangle$. Yet our upper bounds (6a), (7a), and the bound in Ref. [10] are different: no bound is tighter than another in all regimes. To our knowledge, Eqs. (6b) and (7b) are the first lower bounds on thermal states' quantum Fisher information. We compare the bounds in a spin-chain example in Appendix V.

Bounds on single-parameter estimation errors.Consider estimating an unknown parameter $\mu_{l}$. We denote the optimal error by $\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\left.\mu_{l}\right)}\right.}$. The singleparameter quantum Cramér-Rao bound (5) is saturable by suitably chosen estimators [7]. Therefore, Eqs. (6) and (7) engender two sets of upper and lower bounds on $\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right)}$. The relative error $\frac{\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right)}}{\left|\mu_{l}\right|}$ achievable
with $\mathcal{N}$ copies of a thermal state is

$$
\begin{equation*}
\frac{1}{\beta \sqrt{\mathcal{N}} \Delta H_{l}} \leq \frac{\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right)}}{\left|\mu_{l}\right|} \leq \frac{1}{2 \beta c_{1}^{1 / 2} \sqrt{\mathcal{N}} \Delta H_{l}} \tag{9}
\end{equation*}
$$

and

$$
\begin{align*}
& \sqrt{2.4 c_{2}} \beta \sqrt{\mathcal{N}}\left(\left(\Delta H_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, H_{l}\right]\right\|_{2}^{2}\right)^{1 / 2} \\
& \leq \frac{\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right)}}{\left|\mu_{l}\right|} \leq  \tag{10}\\
& \frac{1}{\sqrt{0.8} \beta \sqrt{\mathcal{N}}\left(\left(\Delta H_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, H_{l}\right]\right\|_{2}^{2}\right)^{1 / 2}}
\end{align*}
$$

By Eq. (9), a higher uncertainty $\Delta H_{l}$ in $H_{l}=\mu_{l} A_{l}$ can enable better precision. Meanwhile, Eq. (10) constrains the relative error in terms of the classical uncertainty in $H_{l}=\mu_{l} A_{l}$. Equation (10) also reveals the role of noncommutativity: when $A_{l}$ does not commute with $\rho$, the ability to estimate $\mu_{l}$ diminishes. This fact has an analogue in single-parameter estimation in unitary quantum metrology, as detailed in Appendix III. There, $\mu_{l}$ can be encoded in a probe state via Hamiltonian evolution under $H=\mu_{l} A_{l}+H^{\prime}$, for an arbitrary Hermitian $H^{\prime}$. If $\left[A_{l}, H\right] \neq 0$ - and so $[\rho, H] \neq 0$ for thermal states $\rho$-the ability to measure $\mu_{l}$ is diminished [37].

In quantum metrology, the estimation error's scaling with a sensor's size can constitute an entanglement advantage. Consider a system of $n$ subsystems and $H_{l}$ a sum of $n$ local terms. Superextensive variances $\left(\Delta H_{l}\right)^{2} \sim n^{\alpha}$, with $\alpha>1$, are atypical for thermal states of spatially-local Hamiltonians. For instance, $\left(\Delta H_{l}\right)^{2} \sim n$ for states with exponentially decaying correlations [38, 39]. From Eq. (9), one would expect the optimal estimation error to scale as $1 /(\beta \sqrt{\mathcal{N}} \sqrt{n})$, as in the standard quantum limit [40, 41]. At critical points, however, $\left(\Delta H_{l}\right)^{2} \sim n$ may be violated [15, 42, 43]. We can observe violations also with certain nonlocal Hamiltonians.

We now show that one can beat the standard quantum limit in Hamiltonian metrology using thermal states. Consider estimating a field $\mu$ by measuring copies of a thermal state of the $n$-qubit Hamiltonian $H=\mu \sum_{j=1}^{n}\left(\sigma_{z}^{j}+1\right)-\lambda \bigotimes_{j=1}^{n} n \sigma_{x}^{j} \equiv H_{\mu}+H_{\lambda}$. We assume $\lambda>0$ and $\mu>0$. Let $|\overline{0}\rangle$ denote the $n$-fold tensor product of the eigenvalue- $(-1)$ eigenstate of $\sigma_{z}$; and $|\overline{1}\rangle$, the product of the eigenvalue- 1 eigenstate. The $n$-qubit GHZ state $|\Phi\rangle:=(|\overline{0}\rangle+|\overline{1}\rangle) / \sqrt{2}$ is a ground state of $H_{\lambda}$. We prove in Appendix VI that $|\Phi\rangle$ is the unique ground state if $H_{\mu}$ is a perturbation $(\mu / \lambda \ll 1)$. The variance of $H_{\mu}$ in $|\Phi\rangle$ is $\langle\Phi| H_{\mu}^{2}|\Phi\rangle-\langle\Phi| H_{\mu}|\Phi\rangle^{2}=\mu^{2} n^{2}$. Therefore, one might expect that $\Delta H_{\mu} \sim \mu n^{\alpha}$, with $\alpha>1 / 2$, in lowtemperature thermal states. In Appendix VI, we prove this expectation, showing that $\alpha=1$ for $\beta \lambda n \gg 1$. Note

Relative estimation error vs. number of qubits


FIG. 2. Beating the standard quantum limit. The figure shows the relative estimation error $\sqrt{\operatorname{var}_{\mathrm{opt}}(\hat{\mu})} /|\mu|$ for the parameter $\mu$ in the $n$-qubit $H=\mu \sum_{j}^{n}\left(\sigma_{z}^{j}+1\right)-\lambda \bigotimes_{j}^{n} n \sigma_{x}^{j}:=H_{\mu}+H_{\lambda}$. The bounds appear in Eqs. (9) and (10) [the upper bound in (9) is, here, too loose to appear in the plotted range]. We take $\lambda \beta=2 \mu \beta=6$. As we show in Appendix VI, $\Delta H_{\mu} \sim \mu n$, for large $\beta \lambda n$. A consequence, suggested by Eqs. (9) and (10), is an optimal estimation error that decays faster than $1 / \sqrt{n}$.
this proof does not require that $\mu / \lambda \ll 1$. By Eqs. (9) and (10), this result suggests a minimum relative estimation error that decreases faster than the standard quantum limit $1 / \sqrt{n}$. Figure 2 supports this argument, exhibiting a regime with optimal relative estimation errors below $1 / \sqrt{n}$. These results would have been difficult to deduce from the expression (4) for the quantum Fisher information. By leveraging our bounds, we found a model that beats the standard quantum limit.

Bounds on multiparameter estimation errors.-The single-parameter bounds above apply when all parameters except the target parameter are known. However, our results imply bounds on the error in joint estimates of $M$ Hamiltonian parameters. The variances' sum serves as the error measure. We aim for a total error $\sum_{l=1}^{M} \operatorname{var}\left(\hat{\mu}_{l}\right)=\epsilon_{\text {err }}^{2}$. By the multiparameter CramérRao bound (3),

$$
\begin{equation*}
\epsilon_{\mathrm{err}}^{2}=\sum_{l=1}^{M} \operatorname{var}\left(\hat{\mu}_{l}\right) \geq \frac{1}{\mathcal{N}} \operatorname{Tr}\left(\mathcal{F}^{-1}\right) \geq \frac{1}{\mathcal{N}} \sum_{l=1}^{M} \frac{1}{\mathcal{F}_{l l}} \tag{11}
\end{equation*}
$$

The final inequality holds under the condition $\mathcal{F}>0$, satisfied if one can estimate every linear combination of parameters [6]. The second inequality is useful for large $M$, when calculating $\mathcal{F}^{-1}$ is computationally hard.

The second inequality is saturated if and only if $\mathcal{F}$ is diagonal. The first inequality is saturated if and only if

$$
\begin{align*}
0 & =\operatorname{Tr}\left(\rho\left[L_{l}, L_{m}\right]\right)  \tag{12}\\
& =4 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)^{3}}{\left(\omega_{j}-\omega_{k}\right)^{2}\left(p_{j}+p_{k}\right)^{2}}\langle j| A_{l}|k\rangle\langle k| A_{m}|j\rangle
\end{align*}
$$

for all $\{l, m\}$, where $p_{j}=e^{-\beta \omega_{j}} / Z_{\beta}$. These are
rather stringent conditions violated by typical manybody Hamiltonians.

By combining Eq. (11) with the bounds (6a) and (7a), we bound the error in the estimation of multiple Hamiltonian parameters. To learn $M$ Hamiltonian parameters with an error $\epsilon_{\text {err }}$, one needs a number $\mathcal{N}$ of measurements satisfying

$$
\begin{align*}
& \mathcal{N} \geq \frac{1}{\beta^{2} \epsilon_{\text {err }}^{2}} \sum_{l=1}^{M} \frac{c_{2}^{-1} / 2}{\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}} \quad \text { and }  \tag{13a}\\
& \mathcal{N} \geq \frac{1}{\beta^{2} \epsilon_{\text {err }}^{2}} \sum_{l=1}^{M} \frac{1}{\left(\Delta A_{l}\right)^{2}} \tag{13b}
\end{align*}
$$

Consequently,

$$
\begin{equation*}
\mathcal{N}=\Omega\left(\frac{M}{\beta^{2} \epsilon_{\text {err }}^{2}} \min _{l} \frac{1}{\left(\Delta A_{l}\right)^{2}}\right) \tag{14}
\end{equation*}
$$

We can compare Eq. (14) to complexity-theoretic results $[25,26]$ about the number $\mathcal{N}$ of copies of the state required to learn $M$ Hamiltonian parameters to within an $l_{2}$-distance error $\epsilon$ defined through $\epsilon^{2}=\sum_{l=1}^{M}\left(\hat{\mu}_{l}-\mu_{l}\right)^{2}$. At least $\mathcal{N}=\Omega\left(\frac{\exp (\beta) M}{\beta^{2} \epsilon^{2}}\right)$ samples are required for an $M$-qubit Hamiltonian [26]. At low temperatures, their bound is tighter, as a function of $\beta$. Moreover, we have only proven Eq. (13) to be saturable under stringent conditions on the operators $A_{l}$. They prove a stronger result: $\mathcal{N}=\mathcal{O}\left(\frac{M}{\beta^{2} \epsilon^{2}} \ln (M / \delta)\right)$ samples suffice to learn the parameters with a constant failure probability $\delta$. In contrast, our results are more general since they concern the average error in estimations of parameters in arbitrary Hamiltonians. Also, our results reveal the roles of uncertainties $\Delta A_{l}$, and of the state's noncommutativity with $A_{l}$, in the estimation error. We compare this Letter's bounds with previous bounds in detail in Appendix VIII (see Table I).

Estimation of chemical potentials. - In the presence of conserved charges $Q_{l}$, thermalizing systems reach generalized Gibbs states [44-47]

$$
\begin{equation*}
\rho_{\beta,\left\{\mu_{l}\right\}}=e^{-\beta\left(H_{0}+\sum_{l} \mu_{l} Q_{l}\right)} / Z_{\beta,\left\{\mu_{l}\right\}} \tag{15}
\end{equation*}
$$

$H_{0}$ is the system Hamiltonian. The $\mu_{l}$ are the chemical potentials corresponding to the charges, which satisfy $\left[H_{0}, Q_{l}\right]=0$ for all $l$.

Our results imply constraints on the minimum error in estimations of the chemical potentials: we identify $H \equiv H_{0}+\sum_{l} \mu_{l} Q_{l}$ and $A_{l} \equiv Q_{l}$ in Eq. (1). For example, consider estimating one $\mu_{l}$. Equations (7), with
the quantum Cramér-Rao bound's saturability, imply

$$
\begin{align*}
& \frac{1}{2.4 c_{2} \beta^{2} \mathcal{N}\left(\left(\Delta Q_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, Q_{l}\right]\right\|_{2}^{2}\right)} \\
& \leq \operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right) \leq  \tag{16}\\
& \frac{1}{0.8 \beta^{2} \mathcal{N}\left(\left(\Delta Q_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, Q_{l}\right]\right\|_{2}^{2}\right)}
\end{align*}
$$

Classically, all charges commute with each other and so with $\rho$. Quantum charges can defy this expectation: $\left[Q_{l}, Q_{m}\right] \neq 0[45,46,48-50]$. For instance, the two-qubit Hamiltonian $H_{0}=\sigma_{z} \otimes \sigma_{z}$ conserves charges $Q_{1}=\sigma_{z} \otimes \mathbb{1}$ and $Q_{2}=\sigma_{x} \otimes \sigma_{x}$ that do not commute with each other. This noncommutation prevents charges from commuting with the state: $\left[Q_{l}, \sqrt{\rho}\right] \neq 0$. This lack of equality implies a quantum disadvantage in parameter estimation: charges' noncommutativity hinders the ability to measure chemical potential $\mu_{1}$.

Discussion. - Our bounds highlight how estimation error depends on the noncommutativity of the operators defining the Hamiltonian. The noncommutativity engenders a disadvantage, diminishing precision. See Eq. (10) and Appendix III for a comparison with the estimation of parameters from Hamiltonian evolution.

Furthermore, we found that noncommutativity of conserved charges hinders estimations of chemical potentials. This result contrasts with Refs. [49, 51], which show that conserved quantities' noncommutativity provides an advantage in quantum transport processes by decreasing entropy production. Our work therefore contributes to the debate about whether noncommuting charges enhance or hinder desirable properties in information-processing and thermodynamic tasks [29, 52].

A natural open problem, unexplored in this work, is the construction of concrete protocols that saturate the bounds $[53,54]$. Moreover, we found a toy model where, using measurements on a thermal state, one can beat the standard quantum limit for the task of estimating (a component of) a field coupled locally to $n$ qubits. Further work could shed light on whether one can use thermal states also of more-physically-realistic, fully local Hamiltonians to beat the standard quantum limit, possibly by
exploiting criticality [15, 42, 43, 55].
Note added.-Ref. [56], which studies the Hamiltonian learning problem at all temperatures, was posted during the preparation of this manuscript.

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[1] C. W. Helstrom, Quantum detection and estimation theory, Vol. 1 (Springer, 1969) pp. 231-252.
[2] S. L. Braunstein and C. M. Caves, Statistical distance and the geometry of quantum states, Phys. Rev. Lett. 72, 3439 (1994).
[3] Z. Holmes, G. Muraleedharan, R. D. Somma, Y. Subasi, and B. Şahinoğlu, Quantum algorithms from fluctuation theorems: Thermal-state preparation, Quantum 6, 825 (2022).
[4] C.-F. Chen, M. Kastoryano, F. Brandao, and A. Gilyén,

Quantum thermal state preparation, arXiv preprint arXiv:2303.18224 10 (2023).
[5] L. A. Correa, M. Mehboudi, G. Adesso, and A. Sanpera, Individual quantum probes for optimal thermometry, Phys. Rev. Lett. 114, 220405 (2015).
[6] J. Liu, H. Yuan, X.-M. Lu, and X. Wang, Quantum Fisher information matrix and multiparameter estimation, J. Phys. A: Math. Theor. 53, 023001 (2019).
[7] M. G. Paris, Quantum estimation for quantum technology, Int. J. Quantum Inf. 7, 125 (2009).
[8] M. G. A. Paris, Achieving the Landau bound to precision of quantum thermometry in systems with vanishing gap, J. Phys. A: Math. Theor. 49, 03LT02 (2015).
[9] K. V. Hovhannisyan and L. A. Correa, Measuring the temperature of cold many-body quantum systems, Phys. Rev. B 98, 045101 (2018).
[10] H. J. Miller and J. Anders, Energy-temperature uncertainty relation in quantum thermodynamics, Nat. Commun. 9, 2203 (2018).
[11] P. P. Potts, J. B. Brask, and N. Brunner, Fundamental limits on low-temperature quantum thermometry with finite resolution, Quantum 3, 161 (2019).
[12] W.-K. Mok, K. Bharti, L.-C. Kwek, and A. Bayat, Optimal probes for global quantum thermometry, Commun. Phys. 4, 62 (2021).
[13] M. Mehboudi, M. R. Jørgensen, S. Seah, J. B. Brask, J. Kołodyński, and M. Perarnau-Llobet, Fundamental limits in bayesian thermometry and attainability via adaptive strategies, Phys. Rev. Lett. 128, 130502 (2022).
[14] P. Zanardi, L. Campos Venuti, and P. Giorda, Bures metric over thermal state manifolds and quantum criticality, Phys. Rev. A 76, 062318 (2007).
[15] P. Zanardi, M. G. A. Paris, and L. Campos Venuti, Quantum criticality as a resource for quantum estimation, Phys. Rev. A 78, 042105 (2008).
[16] J. R. Garrison and T. Grover, Does a single eigenstate encode the full Hamiltonian?, Phys. Rev. X 8, 021026 (2018).
[17] M. Greiter, V. Schnells, and R. Thomale, Method to identify parent Hamiltonians for trial states, Phys. Rev. B 98, 081113 (2018).
[18] E. Chertkov and B. K. Clark, Computational inverse method for constructing spaces of quantum models from wave functions, Phys. Rev. X 8, 031029 (2018).
[19] W. Zhu, Z. Huang, and Y.-C. He, Reconstructing entanglement Hamiltonian via entanglement eigenstates, Phys. Rev. B 99, 235109 (2019).
[20] X.-L. Qi and D. Ranard, Determining a local Hamiltonian from a single eigenstate, Quantum 3, 159 (2019).
[21] X. Turkeshi, T. Mendes-Santos, G. Giudici, and M. Dalmonte, Entanglement-guided search for parent Hamiltonians, Phys. Rev. Lett. 122, 150606 (2019).
[22] E. Bairey, I. Arad, and N. H. Lindner, Learning a local Hamiltonian from local measurements, Phys. Rev. Lett. 122, 020504 (2019).
[23] J. Zhou and D. L. Zhou, Recovery of a generic local Hamiltonian from a steady state, Phys. Rev. A 105, 012615 (2022).
[24] K. Rudinger and R. Joynt, Compressed sensing for Hamiltonian reconstruction, Phys. Rev. A 92, 052322 (2015).
[25] A. Anshu, S. Arunachalam, T. Kuwahara, and M. Soleimanifar, Sample-efficient learning of interacting quantum systems, Nat. Phys., 1 (2021).
[26] J. Haah, R. Kothari, and E. Tang, Optimal learning of quantum Hamiltonians from high-temperature Gibbs states, in 2022 IEEE 63rd Annual Symposium on Foundations of Computer Science (FOCS) (IEEE, 2022) pp. 135-146.
[27] A. Gu, L. Cincio, and P. J. Coles, Practical black box Hamiltonian learning, arXiv preprint arXiv:2206.15464 10.48550/arXiv. 2206.15464 (2022).
[28] F. M. Sbahi, A. J. Martinez, S. Patel, D. Saberi, J. H. Yoo, G. Roeder, and G. Verdon, Prov-
ably efficient variational generative modeling of quantum many-body systems via quantum-probabilistic information geometry, arXiv preprint arXiv:2206.04663 10.48550/arXiv. 2206.04663 (2022).
[29] S. Majidy, W. F. Braasch Jr, A. Lasek, T. Upadhyaya, A. Kalev, and N. Yunger Halpern, Noncommuting conserved charges in quantum thermodynamics and beyond, Nat. Rev. Phys. 5, 689 (2023).
[30] E. P. Wigner and M. M. Yanase, Information contents of distributions, PNAS 49, 910 (1963).
[31] S. Luo, Quantum versus classical uncertainty, Theor. Math. Phys. 143, 681 (2005).
[32] S. Luo, Wigner-Yanase skew information and uncertainty relations, Phys. Rev. Lett. 91, 180403 (2003).
[33] J. S. Sidhu and P. Kok, Geometric perspective on quantum parameter estimation, AVS Quantum Sci. 2, 014701 (2020).
[34] I. Marvian and R. W. Spekkens, Extending Noether's theorem by quantifying the asymmetry of quantum states, Nat. Commun. 5, 3821 (2014).
[35] D. Girolami, Observable measure of quantum coherence in finite dimensional systems, Phys. Rev. Lett. 113, 170401 (2014).
[36] D. P. Pires, L. C. Céleri, and D. O. Soares-Pinto, Geometric lower bound for a quantum coherence measure, Phys. Rev. A 91, 042330 (2015).
[37] Of course, in unitary quantum metrology, whether $A_{l}$ commutes with $\sqrt{\rho}$ does not matter: no thermal state will evolve under $H$ and gain information about $\mu_{l}$.
[38] Z. Gong and R. Hamazaki, Bounds in nonequilibrium quantum dynamics, Int. J. Mod. Phys. A 36, 2230007 (2022).
[39] A. M. Alhambra, Quantum many-body systems in thermal equilibrium, PRX Quantum 4, 040201 (2023).
[40] N. Kura and M. Ueda, Standard quantum limit and Heisenberg limit in function estimation, Phys. Rev. Lett. 124, 010507 (2020).
[41] V. Cimini, E. Polino, F. Belliardo, F. Hoch, B. Piccirillo, N. Spagnolo, V. Giovannetti, and F. Sciarrino, Experimental metrology beyond the standard quantum limit for a wide resources range, npj Quantum Inf. 9, 20 (2023).
[42] I. Frérot and T. Roscilde, Quantum critical metrology, Phys. Rev. Lett. 121, 020402 (2018).
[43] M. Gabbrielli, A. Smerzi, and L. Pezzè, Multipartite entanglement at finite temperature, Sci. Rep. 8, 15663 (2018).
[44] L. Vidmar and M. Rigol, Generalized Gibbs ensemble in integrable lattice models, J. Stat. Mech.: Theory Exp. 2016 (6), 064007.
[45] N. Yunger Halpern, P. Faist, J. Oppenheim, and A. Winter, Microcanonical and resource-theoretic derivations of the thermal state of a quantum system with noncommuting charges, Nat. Commun. 7, 1 (2016).
[46] Y. Guryanova, S. Popescu, A. J. Short, R. Silva, and P. Skrzypczyk, Thermodynamics of quantum systems with multiple conserved quantities, Nat. Commun. 7, 12049 (2016).
[47] T. Monnai, Relaxation to generalized Gibbs ensembles in quadratic quantum open systems, JPSJ 89, 124005 (2020).
[48] M. Lostaglio, D. Jennings, and T. Rudolph, Thermodynamic resource theories, non-commutativity and maximum entropy principles, New J. Phys. 19, 043008 (2017).
[49] G. Manzano, J. M. Parrondo, and G. T. Landi, Non-
abelian quantum transport and thermosqueezing effects, PRX Quantum 3, 010304 (2022).
[50] S. Majidy, A. Lasek, D. A. Huse, and N. Yunger Halpern, Non-abelian symmetry can increase entanglement entropy, Phys. Rev. B 107, 045102 (2023).
[51] T. Upadhyaya, W. F. Braasch, G. T. Landi, and N. Yunger Halpern, What happens to entropy production when conserved quantities fail to commute with each other, arXiv (2023), arXiv:2305.15480 [quant-ph].
[52] S. Majidy, A. Lasek, D. A. Huse, and N. Yunger Halpern, Non-abelian symmetry can increase entanglement entropy, Phys. Rev. B 107, 045102 (2023).
[53] Y. L. Len, T. Gefen, A. Retzker, and J. Kołodyński, Quantum metrology with imperfect measurements, Nat. Commun. 13, 6971 (2022).
[54] C. Yin and A. Lucas, Heisenberg-limited metrology with perturbing interactions (2023), arXiv:2308.10929 [quant$\mathrm{ph}]$.
[55] M. Yu, H. C. Nguyen, and S. Nimmrichter, Criticalityenhanced precision in phase thermometry (2023), arXiv:2311.14578 [quant-ph].
[56] A. Bakshi, A. Liu, A. Moitra, and E. Tang, Learning quantum Hamiltonians at any temperature in polynomial time, arXiv (2023), arXiv:2310.02243 [quant-ph].
[57] V. Giovannetti, S. Lloyd, and L. Maccone, Quantum metrology, Phys. Rev. Lett. 96, 010401 (2006).
[58] S. Boixo, A. Datta, S. T. Flammia, A. Shaji, E. Bagan, and C. M. Caves, Quantum-limited metrology with product states, Phys. Rev. A 77, 012317 (2008).
[59] D. Hangleiter, I. Roth, J. Eisert, and P. Roushan, Precise hamiltonian identification of a superconducting quantum processor, arXiv preprint arXiv:2108.08319 (2021).
[60] W. Yu, J. Sun, Z. Han, and X. Yuan, Robust and efficient Hamiltonian learning, Quantum 7, 1045 (2023).
[61] D. S. Franca, L. A. Markovich, V. Dobrovitski, A. H. Werner, and J. Borregaard, Efficient and robust estimation of many-qubit hamiltonians, arXiv preprint arXiv:2205.09567 (2022).
[62] H.-Y. Huang, Y. Tong, D. Fang, and Y. Su, Learning many-body Hamiltonians with heisenberg-limited scaling, Phys. Rev. Lett. 130, 200403 (2023).
[63] J. Wang, S. Paesani, R. Santagati, S. Knauer, A. A. Gentile, N. Wiebe, M. Petruzzella, J. L. O'brien, J. G. Rarity, A. Laing, et al., Experimental quantum Hamiltonian learning, Nat. Phys. 13, 551 (2017).
[64] C. Senko, J. Smith, P. Richerme, A. Lee, W. Campbell, and C. Monroe, Coherent imaging spectroscopy of a quantum many-body spin system, Science 345, 430 (2014).

## APPENDIX

Appendix I - Derivation of the quantum Fisher information matrix of Hamiltonian parameters for thermal states.
Appendix II - Upper and lower bounds on the diagonals of the quantum Fisher information matrix: proof of Eqs. (6) and (7) in the main text.

Appendix III - Role of noncommutativity in parameter estimation.
Appendix IV - Quantum Fisher information of a two-level system.
Appendix V - Comparisons of the bounds on the quantum Fisher information.
Appendix VI - Properties of the Hamiltonian $H=\mu \sum_{j=1}^{n}\left(\sigma_{z}^{j}+1\right)-\lambda \bigotimes_{j=1}^{n} n \sigma_{x}^{j}$.
Appendix VII - Conditions for saturability of the multiparameter Cramér-Rao bound: proof of Eq. (12) in the main text.

Appendix VIII - Comparisons with the literature on Hamiltonian learning.

## I. THE QUANTUM FISHER INFORMATION MATRIX

In this section, we derive the closed-form expression for the quantum Fisher information matrix of Hamiltonian parameters for thermal states.

The quantum Fisher information matrix has elements

$$
\begin{equation*}
\mathcal{F}_{l m}:=2 \sum_{j k} \frac{\operatorname{Re}\left[\langle j| \partial_{l} \rho|k\rangle\langle k| \partial_{m} \rho|j\rangle\right]}{p_{j}+p_{k}} \tag{A1}
\end{equation*}
$$

We have defined $\partial_{l}:=\frac{\partial}{\partial \mu_{l}}$. The matrix characterizes the precision with which multiple parameters $\mu_{l}$ can be estimated. Let $\mathcal{N}$ denote the number of measurements performed. The multiparameter Cramér-Rao bound says that [6]

$$
\begin{equation*}
\operatorname{cov}(\hat{\vec{\mu}}) \geq \frac{1}{\mathcal{N}} \mathcal{F}^{-1} \tag{A2}
\end{equation*}
$$

This bound is asymptotically saturable if and only if

$$
\begin{equation*}
\operatorname{Tr}\left(\rho\left[L_{l}, L_{m}\right]\right)=0 \tag{A3}
\end{equation*}
$$

The symmetric logarithmic derivative is defined by $\partial_{l} \rho=\frac{1}{2}\left\{L_{l}, \rho\right\}$.
Throughout this appendix, we omit the temperature dependence from the partition-function notation: $Z \equiv Z_{\beta}$. Since $\rho=e^{-\beta H} / Z=\sum_{j} e^{-\beta \omega_{j}}|j\rangle\langle j| / Z$, the derivative in Eq. (A1) is

$$
\begin{equation*}
\partial_{l} \rho=\frac{1}{Z} \partial_{l} e^{-\beta H}-\rho \frac{\partial_{l} Z}{Z}=\frac{1}{Z}\left[\partial_{l} e^{-\beta H}-\rho \operatorname{Tr}\left(\partial_{l} e^{-\beta H}\right)\right] . \tag{A4}
\end{equation*}
$$

We must calculate the matrix elements of $\partial_{l} e^{-\beta H}$. Using the Taylor series

$$
\begin{equation*}
e^{-\beta H}=\sum_{n=0}^{\infty}(-\beta)^{n} \frac{H^{n}}{n!} \tag{A5}
\end{equation*}
$$

we obtain

$$
\begin{align*}
\langle j| \partial_{l} e^{-\beta H}|k\rangle & =\sum_{n=0}^{\infty} \frac{(-\beta)^{n}}{n!}\langle j| \partial_{l} H^{n}|k\rangle \\
& =\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!}\langle j| \sum_{m=0}^{n-1} H^{m} A_{l} H^{n-m-1}|k\rangle \\
& =\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} \sum_{m=0}^{n-1} \omega_{j}^{m} \omega_{k}^{n-m-1}\langle j| A_{l}|k\rangle \\
& =\langle j| A_{l}|k\rangle \sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} \sum_{m=0}^{n-1} \omega_{j}^{m} \omega_{k}^{n-m-1} \\
& =\langle j| A_{l}|k\rangle \Gamma_{j k} \tag{A6}
\end{align*}
$$

We have defined

$$
\begin{equation*}
\Gamma_{j k}:=\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} \sum_{m=0}^{n-1} \omega_{j}^{m} \omega_{k}^{n-m-1} \tag{A7}
\end{equation*}
$$

as a function of the temperature and of the Hamiltonian's spectrum.
We can re-express $\Gamma_{j k}$ using the formula for an infinite geometric series: if $\omega_{j} \neq \omega_{k}$, then

$$
\begin{equation*}
\Gamma_{j k}=\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} \frac{\omega_{j}^{n}-\omega_{k}^{n}}{\omega_{j}-\omega_{k}}=\frac{e^{-\beta \omega_{j}}-e^{-\beta \omega_{k}}}{\omega_{j}-\omega_{k}}=Z \frac{\left(p_{j}-p_{k}\right)}{\omega_{j}-\omega_{k}}, \quad \text { for } \quad \omega_{j} \neq \omega_{k} \tag{A8}
\end{equation*}
$$

If $\omega_{j}=\omega_{k}$, then

$$
\begin{align*}
\Gamma_{j k} & =\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} \sum_{m=0}^{n-1} \omega_{j}^{n-1}=\sum_{n=1}^{\infty} \frac{(-\beta)^{n}}{n!} n \omega_{j}^{n-1} \\
& =-\beta \sum_{n=1}^{\infty} \frac{(-\beta)^{n-1}}{(n-1)!} \omega_{j}^{n-1}=-\beta e^{-\beta \omega_{j}} \\
& =-\beta Z p_{j}, \quad \text { for } \quad \omega_{j}=\omega_{k} \tag{A9}
\end{align*}
$$

Using Eqs. (A9) and (A6) we can evaluate the first term in Eq. (A4):

$$
\begin{equation*}
\frac{\operatorname{Tr}\left(\partial_{l} e^{-\beta H}\right)}{Z}=\frac{1}{Z} \sum_{j}\langle j| A_{l}|j\rangle \Gamma_{j j}=-\beta \frac{1}{Z} \sum_{j}\langle j| A_{l}|j\rangle e^{-\beta \omega_{j}}=-\beta\left\langle A_{l}\right\rangle \tag{A10}
\end{equation*}
$$

We denote thermal averages by $\left\langle A_{l}\right\rangle:=\operatorname{Tr}\left(A_{l} \rho\right)$.
Substituting from Eq. (A10) into Eq. (A4) yields

$$
\begin{equation*}
\partial_{l} \rho=\frac{1}{Z} \partial_{l} e^{-\beta H}+\beta\left\langle A_{l}\right\rangle \rho . \tag{A11}
\end{equation*}
$$

Furthermore, substituting into Eq. (A6) from Eqs. (A8) and (A9) yields

$$
\begin{equation*}
\langle j| \partial_{l} e^{-\beta H}|k\rangle=\langle j| A_{l}|k\rangle Z \frac{\left(p_{j}-p_{k}\right)}{\omega_{j}-\omega_{k}}, \quad \text { for } \quad \omega_{j} \neq \omega_{k} \tag{A12}
\end{equation*}
$$

and

$$
\begin{equation*}
\langle j| \partial_{l} e^{-\beta H}|k\rangle=\langle j| A_{l}|k\rangle \Gamma_{j j}=-\langle j| A_{l}|k\rangle \beta Z p_{j} \quad \text { for } \quad \omega_{j}=\omega_{k} \tag{A13}
\end{equation*}
$$

Let $\delta A_{l}:=A_{l}-\left\langle A_{l}\right\rangle=A_{l}-\operatorname{Tr}\left(\rho A_{l}\right)$. If $\omega_{j} \neq \omega_{k}$, then

$$
\begin{equation*}
\langle j| \partial_{l} \rho|k\rangle=\langle j| A_{l}|k\rangle \frac{\left(p_{j}-p_{k}\right)}{\omega_{j}-\omega_{k}}+\beta\left\langle A_{l}\right\rangle\langle j| \rho|k\rangle=\langle j| \delta A_{l}|k\rangle \frac{\left(p_{j}-p_{k}\right)}{\omega_{j}-\omega_{k}}, \quad \text { for } \omega_{j} \neq \omega_{k}, \tag{A14}
\end{equation*}
$$

whereas, if $\omega_{j}=\omega_{k}$,

$$
\begin{equation*}
\langle j| \partial_{l} \rho|k\rangle=-\langle j| A_{l}|k\rangle \beta p_{j}+\beta\left\langle A_{l}\right\rangle p_{j} \delta_{j k}=-\langle j| \delta A_{l}|k\rangle \beta p_{j}=-\langle j| \delta A_{l}|k\rangle \beta \frac{p_{j}+p_{k}}{2}, \quad \text { for } \omega_{j}=\omega_{k} \tag{A15}
\end{equation*}
$$

Thus, the quantum Fisher information matrix in Eq. (A1) becomes

$$
\begin{align*}
\mathcal{F}_{l m} & :=2 \sum_{j k} \frac{\operatorname{Re}\left[\langle j| \partial_{l} \rho|k\rangle\langle k| \partial_{m} \rho|j\rangle\right]}{p_{j}+p_{k}} \\
& =2 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)^{2}}{\left(p_{j}+p_{k}\right)\left(\omega_{j}-\omega_{k}\right)^{2}} \operatorname{Re}\left[\delta A_{j k}^{l} \delta A_{k j}^{m}\right]+\sum_{\omega_{j}=\omega_{k}} \beta^{2} \frac{p_{j}+p_{k}}{2} \operatorname{Re}\left[\delta A_{j k}^{l} \delta A_{k j}^{m}\right] \\
& =2 \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)} \operatorname{Re}\left[\delta A_{j k}^{l} \delta A_{k j}^{m}\right]+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2} \operatorname{Re}\left[\delta A_{j k}^{l} \delta A_{k j}^{m}\right] . \tag{A16}
\end{align*}
$$

In Appendix II, we use this expression to upper- and lower-bound $\mathcal{F}_{l l}$.

## II. BOUNDS ON THE QUANTUM FISHER INFORMATION

In this section, we upper- and lower-bound the diagonals of the quantum Fisher information matrix. That is, we prove Eqs. (6) and (7) from the main text. By Eq. (A16), the quantum Fisher information about a parameter $\mu_{l}$ is

$$
\begin{equation*}
\mathcal{F}_{l l}=2 \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \tag{A17}
\end{equation*}
$$

## Upper bound in terms of $\left(\Delta A_{l}\right)^{2}$

If $x:=p_{k} / p_{j}$, the first term in the quantum Fisher information [Eq. (A17)] depends on $\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)}$. It will be convenient to upper-bound this fraction as $\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)} \leq(1+x) c_{1}$, for some $c_{1}$ to be determined. Shifting the $(1+x)$ from the inequality's right-hand side to the left-hand side, we form a fraction $\frac{(1-x)^{2}}{(1+x)^{2} \ln ^{2}(x)}$ that is maximized at $x=1$. Furthermore, $p_{k} / p_{j}$ comes closest to 1 for energy eigenstates whose energies are as close as possible: $x_{\text {max }}:=e^{-\beta \min _{j, k}\left\{\omega_{k}-\omega_{j}\right\}} \equiv e^{-\beta g_{\text {min }}}$. We have defined $g_{\min }:=\min _{j, k}\left\{\omega_{j}-\omega_{k}\right\}$ as the Hamiltonian's minimum energy gap. Combining these observations, we choose

$$
\begin{equation*}
c_{1}\left(g_{\min }\right):=\frac{\left(1-x_{\max }\right)^{2}}{\left(1+x_{\max }\right)^{2} \ln ^{2}\left(x_{\max }\right)}=\frac{\left(1-e^{-\beta g_{\min }}\right)^{2}}{\left(1+e^{-\beta g_{\min }}\right)^{2}} \frac{1}{\beta^{2} g_{\min }^{2}}=\frac{\tanh ^{2}\left(\beta g_{\min } / 2\right)}{\beta^{2} g_{\min }^{2}} \tag{A18}
\end{equation*}
$$

The limiting values of $c_{1}$, as a function of temperature, are

$$
c_{1}\left(g_{\min }\right) \approx\left\{\begin{array}{lcc}
\frac{1}{\beta^{2} g_{\min }^{2}} & \text { for } \quad \beta g_{\min } \gg 1  \tag{A19}\\
\frac{1}{4} \quad \text { for } & \beta g_{\min } \ll 1
\end{array}\right.
$$

Applying this choice and the general bound above to Eq. (A17), we bound the quantum Fisher information about a parameter $\mu_{l}$ :

$$
\begin{align*}
\mathcal{F}_{l l} & =2 \sum_{\omega_{j} \neq \omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& \leq 2 c_{1}\left(g_{\min }\right) \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} p_{j}\left(1+\frac{p_{k}}{p_{j}}\right)\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2}  \tag{A20a}\\
& =4 c_{1}\left(g_{\min }\right) \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2}+4 c_{1}\left(g_{\min }\right) \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2}+\left[1-4 c_{1}\left(g_{\min }\right)\right] \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 c_{1}\left(g_{\min }\right) \beta^{2} \operatorname{Tr}\left(\rho\left[\delta A_{l}\right]^{2}\right)+\left[1-4 c_{1}\left(g_{\min }\right)\right] \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 c_{1}\left(g_{\min }\right) \beta^{2}\left(\Delta A_{l}\right)^{2}+\left[1-4 c_{1}\left(g_{\min }\right)\right] \beta^{2}\left(\Delta A_{l}^{D}\right)^{2} \tag{A20b}
\end{align*}
$$

We have defined $\Delta A=\sqrt{\left\langle A^{2}\right\rangle-\langle A\rangle^{2}}$ as the standard deviation of an operator $A$ in the thermal state. Also, $A_{l}^{D}:=\sum_{\omega_{j}=\omega_{k}}\langle j| A_{l}|k\rangle|k\rangle\langle j|$ is the sum of the block-diagonal elements of the matrix that represents $A_{l}$ relative to the energy eigenbasis. Since $0 \leq c_{1}\left(g_{\min }\right) \leq 1 / 4$ in Eq. (A20b), also,

$$
\begin{equation*}
\mathcal{F}_{l l} \leq \beta^{2}\left(\Delta A_{l}\right)^{2} \tag{A21}
\end{equation*}
$$

We have proved Eq. (6a) in the main text. Bounds (A20b) and (A21) are saturated if $A_{l}$ is diagonal relative to the energy eigenbasis.

## Lower bound in terms of $\left(\Delta A_{l}\right)^{2}$

A similar derivation implies a lower bound on $\mathcal{F}_{l l}$. The function $\frac{(1-x)^{2}}{(1+x)^{2} \ln ^{2}(x)}$ is minimized at $x=0$ and in the limit as $x \rightarrow \infty$. Moreover, $x$ has a minimum value of $x_{\text {min }}:=e^{-\beta\|H\|_{\mathrm{s}}}$, where $\|H\|_{\mathrm{s}}:=\max _{j} \omega_{j}-\min _{j} \omega_{j}$, and a maximum value of $x_{\text {max }}:=e^{\beta\|H\|_{\mathrm{s}}}$. Since $c_{1}\left(-\|H\|_{\mathrm{s}}\right)=c_{1}\left(\|H\|_{\mathrm{s}}\right)$,

$$
\begin{equation*}
\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)} \geq(1+x) c_{1}\left(\|H\|_{\mathrm{s}}\right) \tag{A22}
\end{equation*}
$$

Using Eqs. (A22) and (A17) leads to

$$
\begin{align*}
\mathcal{F}_{l l} & =2 \sum_{\omega_{j} \neq \omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& \geq 2 c_{1}\left(\|H\|_{\mathrm{s}}\right) \sum_{\omega_{j} \neq \omega_{k}} \beta^{2} p_{j}\left(1+\frac{p_{k}}{p_{j}}\right)\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 c_{1}\left(\|H\|_{\mathrm{s}}\right) \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2}+4 c_{1}\left(\|H\|_{\mathrm{s}}\right) \beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2}+\left[1-4 c_{1}\left(\|H\|_{\mathrm{s}}\right)\right] \beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 c_{1}\left(\|H\|_{\mathrm{s}}\right) \beta^{2} \operatorname{Tr}\left(\rho\left(\delta A_{l}\right)^{2}\right)+\left[1-4 c_{1}\left(\|H\|_{\mathrm{s}}\right)\right] \beta^{2} \sum_{j} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 c_{1}\left(\|H\|_{\mathrm{s}}\right) \beta^{2}\left(\Delta A_{l}\right)^{2} \tag{A23}
\end{align*}
$$

We have proved Eq. (6b) in the main text.

## Upper bound in terms of $\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}$

We can obtain a distinct upper bound that depends on the Wigner-Yanase skew information. Beginning with Eq. (A17), we split the sum over $\omega_{j} \neq \omega_{k}$ into $\omega_{j}<\omega_{k}$ and $\omega_{j}>\omega_{k}$ terms. We can then collapse terms due to the symmetry with respect to the interchange $p_{j} \leftrightarrow p_{k}$ :

$$
\begin{align*}
\mathcal{F}_{l l} & =2 \sum_{\omega_{j} \neq \omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& =2 \sum_{\omega_{j}>\omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+2 \sum_{\omega_{j}<\omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{p_{j}+p_{k}}{2}\left|\delta A_{j k}^{l}\right|^{2} \\
& =4 \sum_{\omega_{j}<\omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} . \tag{A24}
\end{align*}
$$

Assume that the energies $\omega_{j}$ are in ascending order, such that $x_{\min } \leq x:=p_{k} / p_{j} \leq 1$, for $j<k$. The first term in (A24) contains a factor of the form $\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)}$, which obeys the upper bound $\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)} \leq c_{2} \sqrt{x}$ for $0 \leq x \leq 1$, for some $c_{2}$. The minimum value of $x$, at an inverse temperature $\beta$, is $x_{\min }:=\min _{\{j, k\}} p_{k} / p_{j}=\min _{\{j, k\}} e^{-\beta\left(\omega_{k}-\omega_{j}\right)}=e^{-\beta\|H\|_{s}}$. Therefore,

$$
\begin{equation*}
c_{2}:=\frac{1}{\beta^{2}\|H\|_{s}^{2}} e^{\frac{1}{2} \beta\|H\|_{s}} \frac{\left(1-e^{-\beta\|H\|_{s}}\right)^{2}}{1+e^{-\beta\|H\|_{s}}}=\frac{2 \sinh \left(\beta\|H\|_{\mathrm{s}} / 2\right) \tanh \left(\beta\|H\|_{\mathrm{s}} / 2\right)}{\beta^{2}\|H\|_{\mathrm{s}}^{2}} \geq 0.42 \tag{A25}
\end{equation*}
$$

The inequality holds because $2 \sinh (x / 2) \tanh (x / 2) / x^{2} \geq 0.42$ (as one can check using, e.g., Mathematica). The limiting values of $c_{2}$, as a function of temperature, are

$$
c_{2} \approx \begin{cases}e^{\frac{1}{2} \beta\|H\|_{s}} /\left(\beta^{2}\|H\|_{s}^{2}\right), & \text { for } \quad \beta\|H\|_{s} \gg 1  \tag{A26}\\ 1 / 2, & \text { for } \quad \beta\|H\|_{s} \ll 1 .\end{cases}
$$

Let us apply Eq. (A25), with the general bound above, to Eq. (A24):

$$
\begin{align*}
\mathcal{F}_{l l} & =4 \sum_{\omega_{j}<\omega_{k}} \beta^{2} p_{j} \frac{\left(1-p_{k} / p_{j}\right)^{2}}{\left(1+p_{k} / p_{j}\right) \ln ^{2}\left(p_{k} / p_{j}\right)}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& \leq 4 c_{2} \sum_{\omega_{j}<\omega_{k}} \beta^{2} p_{j} \sqrt{\frac{p_{k}}{p_{j}}}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& =2 c_{2} \beta^{2} \sum_{\omega_{j}<\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+2 c_{2} \beta^{2} \sum_{\omega_{j}>\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& \leq 2 c_{2} \beta^{2} \sum_{\omega_{j}<\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+2 c_{2} \beta^{2} \sum_{\omega_{j}>\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+\frac{c_{2}}{0.42} \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2}  \tag{A27a}\\
& \leq 2.4 c_{2} \beta^{2} \sum_{\omega_{j}<\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+2.4 c_{2} \beta^{2} \sum_{\omega_{j}>\omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+2.4 c_{2} \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2}  \tag{A27b}\\
& =2.4 c_{2} \beta^{2} \operatorname{Tr}\left(\sqrt{\rho} \delta A_{l} \sqrt{\rho} \delta A_{l}\right) . \tag{A27c}
\end{align*}
$$

In Eqs. (A27a) and (A27b), we invoked $1 \leq c_{2} / 0.42 \leq 2.4 c_{2}$. Since $\operatorname{Tr}\left(\sqrt{\rho} \delta A_{l} \sqrt{\rho} \delta A_{l}\right)=\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}$, we have proved the second upper bound on $\mathcal{F}_{l l}$, Eq. (7) in the main text.

## Lower bound in terms of $\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}$

Our general expression $\frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)}$ obeys the upper bound $\sqrt{x} / 2.5 \leq \frac{(1-x)^{2}}{(1+x) \ln ^{2}(x)}$. Applying this bound to Eq. (A17) yields

$$
\begin{align*}
\mathcal{F}_{l l} & \geq \frac{2}{2.5} \sum_{\omega_{j} \neq \omega_{k}} \beta^{2} p_{j} \sqrt{\frac{p_{k}}{p_{j}}}\left|\delta A_{j k}^{l}\right|^{2}+\beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& \geq 0.8 \beta^{2} \sum_{\omega_{j} \neq \omega_{k}} \sqrt{p_{j}} \sqrt{p_{k}}\left|\delta A_{j k}^{l}\right|^{2}+0.8 \beta^{2} \sum_{\omega_{j}=\omega_{k}} p_{j}\left|\delta A_{j k}^{l}\right|^{2} \\
& =0.8 \beta^{2} \operatorname{Tr}\left(\sqrt{\rho} \delta A_{l} \sqrt{\rho} \delta A_{l}\right) . \tag{A28}
\end{align*}
$$

This result completes the proof of Eq. (7) in the main text.

## III. NONCOMMUTATIVITY AND PARAMETER ESTIMATION

In this section, we discuss the role of noncommutativity in parameter estimation. In Eq. (10) of the main text, we presented an upper and a lower bound on the optimal relative estimation error $\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\left.\mu_{l}\right)}\right.} /\left|\mu_{l}\right|$ with which a parameter $\mu_{l}$ can be estimated from $\mathcal{N}$ copies of a thermal state. We reproduce the bound here for convenience:

$$
\begin{equation*}
\frac{1}{\sqrt{2.4 c_{2}} \beta \sqrt{\mathcal{N}}\left(\left(\Delta H_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, H_{l}\right]\right\|_{2}^{2}\right)^{1 / 2}} \leq \frac{\sqrt{\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right)}}{\left|\mu_{l}\right|} \leq \frac{1}{\sqrt{0.8} \beta \sqrt{\mathcal{N}}\left(\left(\Delta H_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, H_{l}\right]\right\|_{2}^{2}\right)^{1 / 2}} \tag{A29a}
\end{equation*}
$$

Recall that $H_{l}$ is the Hamiltonian term that contains the parameter $\mu_{l}$. Due to the $\left\|\left[\sqrt{\rho}, H_{l}\right]\right\|_{2}$, noncommutativity between the state and $H_{l}$ negatively impacts one's ability to estimate $\mu_{l}$. Here, we elaborate on the role of noncommutativity in estimating a parameter from Hamiltonian evolution (as opposed to from a thermal state).

In the Hamiltonian-evolution setting, we estimate $\mu_{l}$ by evolving a probe state under a Hamiltonian

$$
\begin{equation*}
H=H_{l}+H^{\prime} \equiv \mu_{l} A_{l}+H^{\prime} \tag{A30}
\end{equation*}
$$

for some time $t . A_{l}$ is a Hermitian matrix (the generator of translations associated with $\mu_{l}$ ). $H^{\prime}$ contains all the (possibly time-dependent) terms independent of $\mu_{l}$. In our setting, $H^{\prime}=\sum_{j \neq l} H_{j}$. The time-evolved state $\varrho(t)$ depends on $\mu_{l}$. One can estimate $\mu_{l}$ from properly chosen measurements of copies of $\varrho(t)$. The minimum achievable variance is bounded in the single-parameter quantum Cramér-Rao bound, Eq. (5) in the main text.

The minimal variance can be achieved with a pure probe state $\varrho=|\psi\rangle\langle\psi|$. We have defined $|\psi\rangle=\left(\left|\lambda_{\max }\right\rangle+\right.$ $\left.\left|\lambda_{\min }\right\rangle\right) / \sqrt{2},\left|\lambda_{\max }\right\rangle$ and $\left|\lambda_{\min }\right\rangle$ denoting the eigenstates associated with the maximum and minimum $A_{l}$ eigenvalues, $\lambda_{\max }$ and $\lambda_{\min }$ [57]. Suppose that $\left|\lambda_{\max }\right\rangle$ and $\left|\lambda_{\min }\right\rangle$ are $H^{\prime}$ eigenstates associated with unit eigenvalues:

$$
\begin{equation*}
H^{\prime}\left|\lambda_{\max }\right\rangle=\left|\lambda_{\max }\right\rangle, \quad \text { and } \quad H^{\prime}\left|\lambda_{\min }\right\rangle=\left|\lambda_{\min }\right\rangle \tag{A31}
\end{equation*}
$$

Evolution under $H$ yields a final state $|\psi(t)\rangle=\left(\left|\lambda_{\max }\right\rangle+e^{\left(\lambda_{\max }-\lambda_{\min }\right) \mu_{l} t}\left|\lambda_{\min }\right\rangle\right) / \sqrt{2}$, from which $\mu_{l}$ can be extracted with a variance $\sim\left[t\left(\lambda_{\max }-\lambda_{\min }\right)\right]^{-2}$, which is optimal [58].

The conditions (A31), under which this optimal scheme works, can be replaced with the weaker condition $\left[H^{\prime}, H_{l}\right]=$ $\left[H, H_{l}\right]=0$. From here, we see the connection to Eq. (A29a): for Gibbs states $\rho$, if $\left[H, H_{l}\right]=0$, then $\left[\sqrt{\rho}, H_{l}\right]=0$. Consequently, we see a direct formal connection between the fact that noncommutativity of $H_{l}$ with $H$ negatively impacts the estimation of $\mu_{l}$ through Hamiltonian evolution and the fact that $\left[\sqrt{\rho}, H_{l}\right] \neq 0$ negatively impacts Hamiltonian learning from Gibbs states.

## IV. QUANTUM FISHER INFORMATION OF A TWO-LEVEL SYSTEM

In this section, we calculate the quantum Fisher information about a parameter in a single-qubit Hamiltonian. Consider the Hamiltonian

$$
\begin{equation*}
H=\Omega_{x} \sigma_{x}+\Omega_{z} \sigma_{z}+\mu \sigma_{z}=: \vec{v} \cdot \vec{\sigma} \tag{A32}
\end{equation*}
$$

We have defined the vector $\vec{v}=\left(\Omega_{x}, \Omega_{z}+\mu\right)$ with the norm $v:=\sqrt{\Omega_{x}^{2}+\left(\Omega_{z}+\mu\right)^{2}}$, and $\vec{\sigma}=\left(\sigma_{x}, \sigma_{z}\right)$ is a vector of Pauli matrices. We aim to estimate $\mu$, so $A=\sigma_{z}$. The thermal state is

$$
\begin{equation*}
\rho=\frac{e^{-\beta v \vec{v} \cdot \vec{\sigma} / v}}{Z}=\frac{\cosh (\beta v) \mathbb{1}-\sinh (\beta v) \vec{v} \cdot \vec{\sigma} / v}{Z} \tag{A33}
\end{equation*}
$$

where $Z=2 \cosh (\beta v)$. The Hamiltonian has a seminorm $\|H\|_{s}=2 v$.
We directly calculate the Wigner-Yanase skew information, using $\sqrt{\rho}=e^{-\beta H / 2} / \sqrt{Z}, A=\sigma_{z}$, and Eq. (A33):

$$
\begin{align*}
\frac{1}{2}\|[\sqrt{\rho}, A]\|_{2}^{2} & =\frac{1}{2 Z}\left\|\sinh (\beta v / 2) / v\left[\vec{v} \cdot \vec{\sigma}, \sigma_{z}\right]\right\|_{2}^{2}=\frac{\sinh ^{2}(\beta v / 2)}{2 v^{2} Z}\left\|\Omega_{x}\left[\sigma_{x}, \sigma_{z}\right]\right\|_{2}^{2} \\
& =\frac{\sinh ^{2}(\beta v / 2)}{2 v^{2} Z}\left\|-2 i \Omega_{x} \sigma_{y}\right\|_{2}^{2}=2 \frac{\sinh ^{2}(\beta v / 2)}{v^{2} Z} \operatorname{Tr}\left(\left[-i \Omega_{x} \sigma_{y}\right]\left[i \Omega_{x} \sigma_{y}\right]\right) \\
& =4 \frac{\sinh ^{2}(\beta v / 2)}{v^{2} Z} \Omega_{x}^{2}=4 \frac{\frac{1}{2}(\cosh (\beta v)-1)}{v^{2} Z} \Omega_{x}^{2}=2 \frac{\cosh (\beta v)-1}{2 v^{2} \cosh (\beta v)} \Omega_{x}^{2} \\
& =\frac{1-\operatorname{sech}(\beta v)}{v^{2}} \Omega_{x}^{2} \tag{A34}
\end{align*}
$$

The thermal variance in $\sigma_{z}$ is

$$
\begin{align*}
(\Delta A)^{2} & =\operatorname{Tr}(\rho)-\left[\operatorname{Tr}\left(\rho \sigma_{z}\right)\right]^{2}=1-\left[-\frac{1}{v Z} \sinh (\beta v) \operatorname{Tr}\left(\vec{v} \cdot \vec{\sigma} \sigma_{z}\right)\right]^{2}=1-\frac{4 \sinh ^{2}(\beta v)}{v^{2} Z^{2}}\left(\Omega_{z}+\mu\right)^{2} \\
& =1-\frac{\tanh ^{2}(\beta v)}{v^{2}}\left(\Omega_{z}+\mu\right)^{2} \tag{A35}
\end{align*}
$$

Subtracting Eq. (A34) from (A35) yields

$$
\begin{equation*}
(\Delta A)^{2}-\frac{1}{2}\|[\sqrt{\rho}, A]\|_{2}^{2}=1-\frac{\tanh ^{2}(\beta v)}{v^{2}}\left(\Omega_{z}+\mu\right)^{2}-\frac{1-\operatorname{sech}(\beta v)}{v^{2}} \Omega_{x}^{2} \tag{A36}
\end{equation*}
$$

We can approximate this expression at high and low temperatures. If the temperature is high $(\beta v \ll 1)$, then $\operatorname{sech}(\beta v) \approx 1-(\beta v)^{2} / 2$, and $\tanh (\beta v) \approx \beta v$. Therefore,

$$
\begin{equation*}
(\Delta A)^{2}-\frac{1}{2}\|[\sqrt{\rho}, A]\|_{2}^{2} \approx 1-\beta^{2}\left(\Omega_{z}+\mu\right)^{2}-\frac{\beta^{2}}{2} \Omega_{x}^{2}=1-\frac{\beta^{2}}{2}\left(\Omega_{z}+\mu\right)^{2}-\frac{\beta^{2}}{2} v^{2} \tag{A37}
\end{equation*}
$$

If the temperature is small, $(\beta v \gg 1)$, then $\operatorname{sech}(\beta v) \approx 2 e^{-\beta v}$, and $\tanh (\beta v) \approx 1$. Therefore,

$$
\begin{equation*}
(\Delta A)^{2}-\frac{1}{2}\|[\sqrt{\rho}, A]\|_{2}^{2} \approx 1-\frac{1}{v^{2}}\left(\Omega_{z}+\mu\right)^{2}-\frac{1}{v^{2}} \Omega_{x}^{2}+\frac{2 e^{-\beta v}}{v^{2}} \Omega_{x}^{2}=\frac{2 e^{-\beta v}}{v^{2}} \Omega_{x}^{2} \tag{A38}
\end{equation*}
$$

Meanwhile, $c_{2} \approx 1 / 2$ at high temperature $(\beta v \ll 1)$, whereas $c_{2} \approx e^{\beta\|H\|_{s} / 2} /\left(\beta\|H\|_{s}\right)^{2}=e^{\beta v} /(2 \beta v)^{2}$ for $\beta v \gg 1$.
By Eq. (A37), at high temperatures $\left(\beta\|H\|_{s} \ll 1\right)$ the bounds (7) in the main text become

$$
\begin{align*}
& \mathcal{F} \leq 2.4 c_{2} \beta^{2} \operatorname{Tr}(\sqrt{\rho} \delta A \sqrt{\rho} \delta A) \approx \frac{2.4}{2} \beta^{2}\left(1-\frac{\beta^{2}}{2}\left(\Omega_{z}+\mu\right)^{2}-\frac{\beta^{2}}{2} v^{2}\right) \approx 1.2 \beta^{2}  \tag{A39a}\\
& \mathcal{F} \geq 0.8 \beta^{2} \operatorname{Tr}(\sqrt{\rho} \delta A \sqrt{\rho} \delta A) \approx 0.8 \beta^{2}\left(1-\frac{\beta^{2}}{2}\left(\Omega_{z}+\mu\right)^{2}-\frac{\beta^{2}}{2} v^{2}\right) \approx 0.8 \beta^{2} \tag{A39b}
\end{align*}
$$

By Eq. (A38), at low temperature $\left(\beta\|H\|_{s} \gg 1\right)$ the bounds (7) become

$$
\begin{align*}
& \mathcal{F} \leq 2.4 c_{2} \beta^{2} \operatorname{Tr}(\sqrt{\rho} \delta A \sqrt{\rho} \delta A) \approx 2.4 \frac{e^{\beta v}}{4 v^{2}}\left(\frac{2 e^{-\beta v}}{v^{2}} \Omega_{x}^{2}\right)=1.2 \frac{\Omega_{x}^{2}}{v^{4}}  \tag{A40a}\\
& \mathcal{F} \geq 0.8 \beta^{2} \operatorname{Tr}(\sqrt{\rho} \delta A \sqrt{\rho} \delta A) \approx 0.8 \beta^{2}\left(\frac{2 e^{-\beta v}}{v^{2}} \Omega_{x}^{2}\right)=1.6 \frac{\beta^{2} e^{-\beta v} \Omega_{x}^{2}}{v^{2}} \tag{A40b}
\end{align*}
$$

We want to compare these bounds with the values of the quantum Fisher information. Define the $\sigma_{z}$ eigenstates such that $\sigma_{z}|1\rangle=|1\rangle$ and $\sigma_{z}|0\rangle=-|0\rangle . H=\vec{v} . \vec{\sigma}$ has the eigenvectors
corresponding to eigenvalues $\pm v$. By the expression (A17) for the quantum Fisher information, for a qubit,

$$
\begin{align*}
\mathcal{F} & \left.=2 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)^{2}}{\left(p_{j}+p_{k}\right)\left(\omega_{j}-\omega_{k}\right)^{2}}\left|\delta A_{j k}^{l}\right|^{2}+\sum_{\omega_{j}=\omega_{k}} \beta^{2} p_{j}\left|\langle j| \delta A_{l}\right| k\right\rangle\left.\right|^{2} \\
& \left.\left.\left.=\frac{4}{Z}\left(\frac{\left(e^{-\beta v}-e^{\beta v}\right)^{2}}{\left(e^{-\beta v}+e^{\beta v}\right)(2 v)^{2}}\right)|\langle+| \delta X|-\right\rangle\left.\right|^{2}+\beta^{2} \frac{e^{-\beta v}}{Z}|\langle+| \delta X|+\right\rangle\left.\right|^{2}+\beta^{2} \frac{e^{\beta v}}{Z}|\langle-| \delta X|-\right\rangle\left.\right|^{2} . \tag{A43}
\end{align*}
$$

We evaluate this expression using

$$
\begin{align*}
\langle+| \delta A|-\rangle & =\frac{1}{2 v\left(\Omega_{z}+\mu+v\right)}\left(-\Omega_{x}\left(\Omega_{z}+\mu+v\right)-\Omega_{x}\left(\Omega_{z}+\mu+v\right)\right)=-\frac{\Omega_{x}}{v}  \tag{A44a}\\
\langle+| \delta A|+\rangle & =\frac{1}{2 v\left(\Omega_{z}+\mu+v\right)}\left(\left(\Omega_{z}+\mu+v\right)^{2}-\Omega_{x}^{2}\right)-\left\langle\sigma_{z}\right\rangle:=a-\left\langle\sigma_{z}\right\rangle, \quad \text { and }  \tag{A44b}\\
\langle-| \delta A|-\rangle & =\frac{1}{2 v\left(\Omega_{z}+\mu+v\right)}\left(\Omega_{x}^{2}-\left(\Omega_{z}+\mu+v\right)^{2}\right)-\left\langle\sigma_{z}\right\rangle:=-a-\left\langle\sigma_{z}\right\rangle . \tag{A44c}
\end{align*}
$$

We have defined $a:=\frac{1}{2 v\left(\Omega_{z}+\mu+v\right)}\left(\left(\Omega_{z}+\mu+v\right)^{2}-\Omega_{x}^{2}\right)=\frac{\left(\Omega_{z}+\mu\right)}{v\left(\Omega_{z}+\mu+v\right)}\left(\Omega_{z}+\mu+v\right)=\frac{\left(\Omega_{z}+\mu\right)}{v}$. Next, we evaluate

Eq. (A43) using Eq. (A44), $Z=2 \cosh (\beta v)$, and $\left\langle\sigma_{z}\right\rangle=-\frac{\tanh (\beta v)}{v}\left(\Omega_{z}+\mu\right)$ from Eq. (A35):

$$
\begin{align*}
\mathcal{F} & =\frac{4}{Z}\left(\frac{\left(e^{-\beta v}-e^{\beta v}\right)^{2}}{\left(e^{-\beta v}+e^{\beta v}\right)(2 v)^{2}}\right) \frac{\Omega_{x}^{2}}{v^{2}}+\left(\beta^{2} \frac{e^{-\beta v}}{Z}+\beta^{2} \frac{e^{\beta v}}{Z}\right)\left(a^{2}+\left\langle\sigma_{z}\right\rangle^{2}\right)+\left(\beta^{2} \frac{e^{-\beta v}}{Z}-\beta^{2} \frac{e^{\beta v}}{Z}\right)\left(-2 a\left\langle\sigma_{z}\right\rangle\right) \\
& =\frac{\left(-e^{-\beta v}+e^{\beta v}\right)}{2 \cosh (\beta v)} \tanh (\beta v) \frac{\Omega_{x}^{2}}{v^{4}}+\beta^{2} \frac{e^{-\beta v}+e^{\beta v}}{2 \cosh (\beta v)}\left(a^{2}+\left\langle\sigma_{z}\right\rangle^{2}\right)-\beta^{2} \frac{e^{-\beta v}-e^{\beta v}}{2 \cosh (\beta v)} 2 a\left\langle\sigma_{z}\right\rangle \\
& =\tanh ^{2}(\beta v) \frac{\Omega_{x}^{2}}{v^{4}}+\beta^{2}\left(a^{2}+\left\langle\sigma_{z}\right\rangle^{2}\right)+2 \beta^{2} \tanh (\beta v) a\left\langle\sigma_{z}\right\rangle \\
& =\tanh ^{2}(\beta v) \frac{\Omega_{x}^{2}}{v^{4}}+\beta^{2}\left(\frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}}+\tanh ^{2}(\beta v) \frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}}\right)-2 \beta^{2} \tanh ^{2}(\beta v) \frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}} \\
& =\tanh ^{2}(\beta v) \frac{\Omega_{x}^{2}}{v^{4}}+\beta^{2} \frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}}-\beta^{2} \tanh ^{2}(\beta v) \frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}} \\
& =\tanh ^{2}(\beta v) \frac{\Omega_{x}^{2}}{v^{4}}+\beta^{2} \frac{\left(\Omega_{z}+\mu\right)^{2}}{v^{2}}\left(1-\tanh ^{2}(\beta v)\right) \tag{A45}
\end{align*}
$$

Using that $\tanh (x) \approx x$ for $x \ll 1$ and that $\tanh (x) \approx 1$ for $x \gg 1$ yields

$$
\begin{align*}
\mathcal{F} & \approx \frac{\beta^{2} \Omega_{x}^{2}}{v^{2}}+\frac{\beta^{2}\left(\Omega_{z}+\mu\right)^{2}}{v^{2}}\left(1-\beta^{2} v^{2}\right) \approx \beta^{2}, \quad \text { for } \beta\|H\|_{s} \ll 1, \quad \text { and }  \tag{A46a}\\
\mathcal{F} & \approx \frac{\Omega_{x}^{2}}{v^{4}}, \quad \text { for } \beta\|H\|_{s} \gg 1 \tag{A46b}
\end{align*}
$$

Let us compare the high-temperature upper bound (A39a) with the approximate value (A46a), as well as the lowtemperature upper bound (A40a) with the approximate value (A46b). The main-text upper bound (7) is saturable, to within a constant multiplicative factor, in both temperature regimes. Together with the Cramér-Rao bound, our bounds imply that

$$
\operatorname{var}_{\mathrm{opt}}\left(\hat{\mu}_{l}\right) \approx \begin{cases}\frac{1}{\mathcal{N} \beta^{2}}, & \text { for } \beta\|H\|_{s} \ll 1  \tag{A47}\\ \frac{\|H\|_{s}^{4}}{16 \mathcal{N} \Omega_{x}^{2}}, & \text { for } \beta\|H\|_{s} \gg 1\end{cases}
$$

## V. COMPARISONS OF BOUNDS ON THE QUANTUM FISHER INFORMATION

In this section, we calculate quantum Fisher information in a spin-chain example. We compare the exact value with our bounds, Eqs. (6) and (7) in the main text. We reproduce the bounds here for convenience:

$$
\begin{align*}
& \mathcal{F}_{l l} \leq \beta^{2}\left(\Delta A_{l}\right)^{2}  \tag{A48a}\\
& \mathcal{F}_{l l} \geq 4 \beta^{2} c_{1}\left(\Delta A_{l}\right)^{2} \tag{A48b}
\end{align*}
$$

and

$$
\begin{align*}
& \mathcal{F}_{l l} \leq 2.4 c_{2} \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right)  \tag{A49a}\\
& \mathcal{F}_{l l} \geq 0.8 \beta^{2}\left(\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\|\left[\sqrt{\rho}, A_{l}\right]\right\|_{2}^{2}\right) \tag{A49b}
\end{align*}
$$

We also compare the bounds to the one derived in Ref. [10]:

$$
\begin{equation*}
\mathcal{F}_{l l} \leq \beta^{2} \int_{0}^{1} \operatorname{Tr}\left(\rho^{a} \delta A_{l} \rho^{1-a} \delta A_{l}\right) d a \tag{A50}
\end{equation*}
$$

with $\delta A_{l}:=A_{l}-\left\langle A_{l}\right\rangle$.
Consider estimating the parameter $\mu$ from the thermal state of a spin chain. We consider a one-dimensional chain composed of $n$ spin- $1 / 2$ systems, with the Hamiltonian

$$
\begin{equation*}
H=\mu \sum_{j=1}^{n} \sigma_{z}^{j}+\lambda \sum_{j=1}^{n-1} \sigma_{x}^{j} \otimes \sigma_{x}^{j+1}=: \mu A_{\mu}+\lambda A_{\lambda} \tag{A51}
\end{equation*}
$$

$A_{\mu}$ and $A_{\lambda}$ are the operators that multiply the parameters $\mu$ and $\lambda$.
Figure 3 compares the quantum Fisher information about $\mu$ with the upper and lower bounds in Eqs. (6) and (7), and with the upper bound in Ref. [10]. We simulate $n=5$ spins. The figure shows that the bounds are distinct and that none of them is tighter than another in all regimes: in each subfigure, the two blue curves (upper bounds derived in this Letter) and the orange star plot (bound in Ref. [10]) cross, as do the two red curves (lower bounds derived in this Letter). However, the bounds are always obeyed: the black curve (exactly calculated quantum Fisher information) always lies below the blue curves and orange star plot (upper bounds) and above the red curves (lower bounds).
(a) Quantum Fisher information vs. $\beta(\lambda / \mu=5)$

(b) Quantum Fisher information vs. $\lambda(\beta \mu=0.1)$


FIG. 3. Comparisons of bounds on the quantum Fisher information. The figure shows log-log plots of the quantum Fisher information $\mathcal{F}_{\mu}$ about parameter $\mu$, as a function of the inverse temperature (left) and as a function of the parameter $\Omega$ (right). The 5-qubit system has the Hamiltonian $H=\mu \sum_{j=1}^{n} \sigma_{z}^{j}+\lambda \sum_{j=1}^{n-1} \sigma_{x}^{j} \otimes \sigma_{x}^{j+1}:=\mu A_{\mu}+\lambda A_{\lambda}$. The plots also depict the upper and lower bounds in Eqs. (6) and (7), and the upper bound derived in Ref. [10]. Each plot illustrates (where a red line crosses a red line or a blue line or orange stars cross) how different bounds can be tighter in different regimes.

## VI. A MODEL THAT CAN BEAT THE STANDARD QUANTUM LIMIT

Here, we prove that the Hamiltonian

$$
\begin{equation*}
H=\mu \sum_{j=1}^{n}\left(\sigma_{z}^{j}+1\right)-\lambda \bigotimes_{j=1}^{n} n \sigma_{x}^{j} \equiv H_{\mu}+H_{\lambda} \tag{A52}
\end{equation*}
$$

considered in the main text has the GHZ state as its unique ground state when $\mu \ll \lambda$. We also prove that $\left(\Delta H_{\mu}\right)^{2} \approx \mu^{2} n^{2}$ for $\beta \lambda n \gg 1$.

For convenience, we shift $H_{\mu}$ by an irrelevant factor of $(\mu n) \mathbb{1}$ so that we consider the new Hamiltonian

$$
\begin{equation*}
\widetilde{H}=\mu \sum_{j=1}^{n}\left(\sigma_{z}^{j}+1+n\right)-\lambda \bigotimes_{j=1}^{n} n \sigma_{x}^{j} \equiv \widetilde{H}_{\mu}+H_{\lambda} \tag{A53}
\end{equation*}
$$

In the computational basis, labeled by bit strings $s \in\{0,1\}^{n}$, this Hamiltonian is block diagonal, with $2^{n-1}$ blocks of dimension two spanned by pairs of computational basis states $\{|s\rangle,|\bar{s}\rangle\}$. Here, $\bar{s}$ denotes the complement of $s$-i.e. $\bar{s}_{j}=s_{j}+1(\bmod 2)$. These blocks, each labeled by a bitstring $s$, take the form

$$
\widetilde{H}_{s}=\left[\begin{array}{cc}
\mu z & -\lambda n  \tag{A54}\\
-\lambda n & -\mu z
\end{array}\right]
$$

where $z \equiv 2|\bar{s}|-n$ and $|\bar{s}|$ denotes the Hamming weight (i.e. the number of ones) of the bitstring $\bar{s}$. Note that we have two distinct, but equivalent, choices of the bitstring $s$ that labels each block. Also, $z \in[-n, n]$.

Each such block can be simply diagonalized, and, thus, so can $\widetilde{H}=\bigoplus_{s} \widetilde{H}_{s}$. The eigenvalues of Eq. (A54) are $\pm \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}$. Consequently, the minimum eigenvalue of $\widetilde{H}$ occurs for the block where $|\bar{s}|=0$ (under a different, but equivalent, choice of labeling this block, $|\bar{s}|=n$ ). The associated minimum eigenvalue is $-n \sqrt{\mu^{2}+\lambda^{2}}$ and the corresponding eigenstate (the ground state of $\widetilde{H}$ ) is

$$
\begin{equation*}
|\mathrm{gs}\rangle \propto-\left(\frac{\mu-\sqrt{\mu^{2}+\lambda^{2}}}{\lambda}\right)|s\rangle+|\bar{s}\rangle . \tag{A55}
\end{equation*}
$$

Consequently, for $\mu / \lambda \ll 1$, it holds that $|\mathrm{gs}\rangle \propto|s\rangle+|\bar{s}\rangle$, which is precisely the GHZ state $|\Phi\rangle$.
For the GHZ state, it holds that $\Delta \widetilde{H}_{\mu}=\mu n$. Consequently, we might expect, at least at low temperatures, that the thermal states of this model might also exhibit estimation errors that decrease faster than the standard quantum limit. This expectation can be analytically validated. In particular, a general thermal state takes the form

$$
\begin{equation*}
\rho=Z_{\beta}^{-1} e^{-\beta \widetilde{H}}=Z_{\beta}^{-1} \bigoplus_{s} e^{-\beta \widetilde{H}_{s}} \tag{A56}
\end{equation*}
$$

where $Z_{\beta}$ is the partition function. It is easy to evaluate

$$
\begin{equation*}
e^{-\beta \widetilde{H}_{s}}=\cosh \left(\beta \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}\right) \mathbb{1}-\sinh \left(\beta \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}\right) \frac{(\mu z) \sigma_{z}-(\lambda n) \sigma_{x}}{\sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}} \tag{A57}
\end{equation*}
$$

Consequently,

$$
\begin{equation*}
Z_{\beta}=2 \sum_{s} \cosh \left(\beta \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}\right) . \tag{A58}
\end{equation*}
$$

We can evaluate the variance $\left(\Delta \widetilde{H}_{\mu}\right)^{2}$ as $\sum_{s}\left(\Delta \widetilde{H}_{\mu, s}\right)^{2}$ where $H_{\mu, s}=\mu z \sigma_{z}$ is the block of $H_{\mu}$ labeled by the bit string $s$. In particular,

$$
\begin{align*}
\left(\Delta \widetilde{H}_{\mu, s}\right)^{2} & =\operatorname{Tr}\left[\rho_{s} \widetilde{H}_{\mu, s}^{2}\right]-\operatorname{Tr}\left[\rho_{s} \widetilde{H}_{\mu, s}\right]^{2} \\
& =Z_{\beta}^{-1}\left[2 \mu^{2} z^{2} \cosh \left(\beta \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}\right)-\frac{4 \mu^{4} z^{4} \sinh ^{2}\left(\beta \sqrt{\mu^{2} z^{2}+\lambda^{2} n^{2}}\right)}{Z_{\beta}\left(\mu^{2} z^{2}+\lambda^{2} n^{2}\right)}\right] \tag{A59}
\end{align*}
$$

where we used that $\rho_{s}=Z_{\beta}^{-1} e^{-\beta \widetilde{H}_{s}}\left(\right.$ note, $\left.\rho=\bigoplus_{s} \rho_{s}\right)$.
Asymptotically in $\beta \lambda n$, we only have to consider the $z=n$ block in Eqs. (A58)-(A59), as $\lim _{x \rightarrow \infty} \frac{\cosh ((1+\epsilon) x)}{\cosh (x)}=\infty$ (also, $\left.\lim _{x \rightarrow \infty} \frac{\sinh ((1+\epsilon) x)}{\sinh (x)}=\infty\right)$ for any $\epsilon>0$. Consequently, asymptotically in $\beta \lambda n$,

$$
\begin{align*}
\left(\Delta \widetilde{H}_{\mu}\right)^{2} & \sim \frac{1}{2 \cosh \left(\beta n \sqrt{\mu^{2}+\lambda^{2}}\right)}\left[2 \mu^{2} n^{2} \cosh \left(\beta n \sqrt{\mu^{2}+\lambda^{2}}\right)-\frac{2 \mu^{4} n^{4} \sinh ^{2}\left(\beta n \sqrt{\mu^{2}+\lambda^{2}}\right)}{n^{2} \cosh \left(\beta n \sqrt{\mu^{2}+\lambda^{2}}\right)\left(\mu^{2}+\lambda^{2}\right)}\right] \\
& =\mu^{2} n^{2}-\tanh ^{2}\left(\beta n \sqrt{\mu^{2}+\lambda^{2}}\right) \frac{\mu^{4} n^{2}}{\mu^{2}+\lambda^{2}} \\
& \sim \mu^{2} n^{2}\left(1-\frac{\mu^{2}}{\mu^{2}+\lambda^{2}}\right) \tag{A60}
\end{align*}
$$

where, in the last line, we use that $\beta>0$. Therefore, we find the scaling $\left(\Delta \widetilde{H}_{\mu}\right)^{2} \sim \mu^{2} n^{2}$ for $\beta \lambda n \gg 1-$ up to subleading, constant factor contributions to the scaling that depend on $\lambda$. Since shifts by constants do not change the variance of an operator, this also implies that $\left(\Delta H_{\mu}\right)^{2} \sim \mu^{2} n^{2}$

## VII. SATURABILITY OF THE MULTIPARAMETER CRAMÉR-RAO BOUND

In this section, we derive conditions under which the multiparameter Cramér-Rao bound is saturated. That is, we prove Eq. (12) in the main text. The multiparameter Cramér-Rao bound is saturable if and only if [6]

$$
\begin{equation*}
\operatorname{Tr}\left(\rho\left[L_{l}, L_{m}\right]\right)=0 \tag{A61}
\end{equation*}
$$

To calculate this equation's left-hand side, we express the trace relative to the $\rho$ eigenbasis. Relative to that eigenbasis, the symmetric logarithmic derivative is represented by a matrix with elements [6]

$$
\begin{equation*}
\langle j| L_{l}|k\rangle=2 \frac{\langle j| \partial_{l} \rho|k\rangle}{p_{j}+p_{k}} \tag{A62}
\end{equation*}
$$

After substituting into the trace, we invoke Eqs. (A14) and (A15):

$$
\begin{align*}
\operatorname{Tr}\left(\rho\left[L_{l}, L_{m}\right]\right) & =\sum_{j k}\left(p_{j}\langle j| L_{l}|k\rangle\langle k| L_{m}|j\rangle-p_{k}\langle k| L_{m}|j\rangle\langle j| L_{l}|k\rangle\right)=\sum_{j k}\left(p_{j}-p_{k}\right)\langle j| L_{l}|k\rangle\langle k| L_{m}|j\rangle \\
& =4 \sum_{j k} \frac{\left(p_{j}-p_{k}\right)}{\left(p_{j}+p_{k}\right)^{2}}\langle j| \partial_{l} \rho|k\rangle\langle k| \partial_{m} \rho|j\rangle \\
& =4 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)}{\left(p_{j}+p_{k}\right)^{2}}\langle j| \delta A_{l}|k\rangle\langle k| \delta A_{m}|j\rangle \frac{\left(p_{j}-p_{k}\right)^{2}}{\left(\omega_{j}-\omega_{k}\right)^{2}} \\
& +4 \beta^{2} \sum_{\omega_{j}=\omega_{k}} \frac{\left(p_{j}-p_{k}\right)}{\left(p_{j}+p_{k}\right)^{2}}\langle j| \delta A_{l}|k\rangle\langle k| \delta A_{m}|j\rangle p_{j}^{2} \\
& =4 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)^{3}}{\left(\omega_{j}-\omega_{k}\right)^{2}\left(p_{j}+p_{k}\right)^{2}}\langle j| A_{l}|k\rangle\langle k| A_{m}|j\rangle . \tag{A63}
\end{align*}
$$

This expression and Eq. (A61) imply Eq. (12) in the main text.
In typical Hamiltonians, most parameters will not satisfy the rather stringent conditions (12) for saturation. They are satisfied, for example, when the operators $A_{l}$ are diagonal relative to the energy eigenbasis. Hence the multiparameter Cramér-Rao bound is saturable when one is estimating the Hamiltonian eigenvalues $\omega_{j}$.

The single parameter Cramér-Rao bound can be saturated with measurements in the eigenbasis of the symmetric logarithmic derivative $L_{l}$ in Eq. (A64) [7]. Using Eqs. (A14) and (A15) into Eq. (A62), we find that

$$
\begin{align*}
L_{l} & =\sum_{\omega_{j} \neq \omega_{k}} 2 \frac{\langle j| \partial_{l} \rho|k\rangle}{p_{j}+p_{k}}|j\rangle\langle k|+\sum_{\omega_{j}=\omega_{k}} 2 \frac{\langle j| \partial_{l} \rho|k\rangle}{2 p_{j}}|k\rangle\langle j| \\
& =2 \sum_{\omega_{j} \neq \omega_{k}} \frac{\left(p_{j}-p_{k}\right)}{\left(p_{j}+p_{k}\right)\left(\omega_{j}-\omega_{k}\right)}\langle j| \delta A_{l}|k\rangle|j\rangle\langle k|-\beta \sum_{\omega_{j}=\omega_{k}}\langle j| \delta A_{l}|k\rangle|k\rangle\langle j| \tag{A64}
\end{align*}
$$

Performing measurements on the eigenbasis of $L_{l}$ would yield one protocol to saturate the Cramér-Rao bound.

## VIII. COMPARISONS WITH THE HAMILTONIAN-LEARNING LITERATURE

In this section, we compare our bounds to earlier results concerning the Hamiltonian-learning problem. Two approaches to Hamiltonian learning are common: (i) the steady-state-based approach and (ii) the time-evolutionbased approach. In the steady-state-based approach, one studies states $\rho$ that are stationary with respect to evolution under the Hamiltonian $H$. These steady states satisfy the condition [22]

$$
\partial_{t} \rho=-i[H, \rho]=0
$$

Every Hamiltonian eigenstate is a steady state, as is the Gibbs state, $\frac{\exp (-\beta H)}{\operatorname{Tr}(\exp (-\beta H))}$. Several studies concern estimations of the Hamiltonian from eigenstates [16-23] or from Gibbs states [22, 25-28].

In the time-evolution-based approach, one analyzes the system's time evolution under the Hamiltonian. Several proposals concern learning the Hamiltonian from unitary dynamics [27, 59-62]. Experimental implementations [63, 64] of Hamiltonian-learning protocols have been carried out, too. In the Hamiltonian-learning problem, one aims to learn the Hamiltonian $H$ from a physically relevant class of Hamiltonians, while minimizing the algorithm's run time and the number of copies of $\rho$. These two metrics are commonly known as sample complexity and time complexity, respectively.

In this work, we focus on learning about a Hamiltonian from Gibbs states. Our comparison of sample-complexity lower bounds with earlier works is presented in the context of the $l_{2}$ distance error, defined via $\epsilon=\left(\sum_{l=1}^{M}\left|\mu_{l}-\hat{\mu}_{l}\right|^{2}\right)^{\frac{1}{2}}$. Here, $\hat{\mu}_{l}$ denotes the estimate for $\mu_{l}$. The rationale for this comparison criterion is due to our adoption of the related metric $\epsilon_{\text {err }}$, defined via $\sum_{l=1}^{M} \operatorname{var}\left(\hat{\mu}_{l}\right)=\epsilon_{\text {err }}^{2}$. We provide the following Lemma to relate the two error metrics.

Lemma 1. For $\epsilon$ and $\epsilon_{\text {err }}$ defined as before, the following holds.

1. $\operatorname{Prob}\left(\epsilon^{2} \geq a\right) \leq \frac{\epsilon_{\text {err }}^{2}}{a}$ for all $a>0$.
2. $\operatorname{Prob}\left(\left|\epsilon^{2}-\epsilon_{e r r}^{2}\right| \geq a\right) \leq \frac{\operatorname{Var}\left(\epsilon^{2}\right)}{a}$ for all $a>0$.
3. For any two real numbers $b$ and $a$ such that $b \geq a$, let $\operatorname{Prob}\left(a \leq \epsilon^{2} \leq b\right)=1$. Then $a \leq \epsilon_{e r r}^{2} \leq b$.

Proof. (Proof of part 1) Note that $\epsilon_{\mathrm{err}}^{2}=\sum_{l=1}^{M} \operatorname{var}\left(\hat{\mu_{l}}\right)$ and $\epsilon^{2}=\sum_{l=1}^{M}\left(\hat{\mu}_{l}-\mu_{l}\right)^{2}$. Since $\hat{\mu_{l}}$ is an unbiased estimator for $\mu_{l}$, we have $\mathbb{E}\left(\hat{\mu}_{l}\right)=\mu_{l}$ for $l \in\{1,2, \cdots, M\}$.

Thus,

$$
\begin{equation*}
\operatorname{var}\left(\hat{\mu}_{l}\right)=\mathbb{E}\left[\left(\hat{\mu_{l}}-\mathbb{E}\left(\hat{\mu_{l}}\right)\right)^{2}\right]=\mathbb{E}\left[\left(\hat{\mu_{l}}-\mu_{l}\right)^{2}\right] \tag{A65}
\end{equation*}
$$

Let us define a new random variable, $V_{l}=\left(\hat{\mu_{l}}-\mu_{l}\right)^{2}$. Thus, using Eq. (A65), we get

$$
\begin{equation*}
\epsilon_{\mathrm{err}}^{2}=\sum_{l=1}^{M} \mathbb{E}\left[V_{l}\right] \tag{A66}
\end{equation*}
$$

and

$$
\begin{equation*}
\epsilon^{2}=\sum_{l=1}^{M} V_{l} \tag{A67}
\end{equation*}
$$

Since $V_{l}$ is a non-negative random variable, using Markov's inequality with Eqs. (A66) and (A67), we get

$$
\operatorname{Prob}\left(\epsilon^{2} \geq a\right) \leq \frac{\epsilon_{\mathrm{err}}^{2}}{a}
$$

for $a>0$. This completes the proof of part 1 .
(Proof of part 2) If $Y$ is a random variable with $\mathbb{E}(Y)=\alpha$ and $\operatorname{Var}(Y)=\beta$, Chebyshev's inequality says

$$
\operatorname{Prob}(|Y-\alpha| \geq a) \leq \frac{\beta}{a} \quad \forall a>0
$$

Applying Chebyshev's inequality to $Y=\epsilon^{2}=\sum_{l=1}^{M} V_{l}$, we get

$$
\begin{equation*}
\operatorname{Prob}\left(\left|\epsilon^{2}-\alpha\right| \geq a\right) \leq \frac{\operatorname{Var}\left(\epsilon^{2}\right)}{a} \quad \forall a>0 \tag{A68}
\end{equation*}
$$

Since expectation is linear, we have

$$
\begin{equation*}
\alpha=\mathbb{E}\left(\epsilon^{2}\right)=\epsilon_{\mathrm{err}}^{2} \tag{A69}
\end{equation*}
$$

Using Eqs. (A68) and (A69), we get the desired result.
(Proof of part 3) For any random variable $Z$ and two real numbers $a, b$ such that $b \geq a$, the following holds:

$$
\begin{equation*}
\operatorname{Prob}(a \leq Z \leq b)=1 \Longrightarrow a \leq \mathbb{E}(Z) \leq b \tag{A70}
\end{equation*}
$$

Substituting $Z=\epsilon^{2}$ in Eq. (A70) and using Eq. (A69) for the expectation value of $Z$, we get the desired result.
Distinctly from prior findings, our sample-complexity lower bound is defined by the commutativity of the Gibbs state with the terms in the Hamiltonian. Our approach relies on no assumptions about the Hamiltonian's structure. In contrast, earlier studies focused on low-interaction Hamiltonians: each term in the Hamiltonian is supported on a constant number of qubits. For a synopsis, refer to Table I.

| Reference | Sample-complexity lower bound | Key technique |
| :---: | :---: | :---: |
| Bairey et al. $[22]$ | $?$ | NA |
| Anshu et al. $[25]$ | $\Omega\left(\frac{\sqrt{M}+\log (1-\delta)}{\beta \epsilon}\right)$ | Quantum state discrimination |
| Sbahi et al. $[28]$ | $?$ | NA |
| Haah et al. $[26]$ | $\Omega\left(\frac{\exp (\beta) M}{\beta^{2} \epsilon^{2}}\right)$ | Coding theory |
| Gu et al. $[27]$ | $?$ | NA |
| This work | $\Omega\left(\frac{M}{\beta^{2} \epsilon_{\text {err }}^{2}} \max \left\{\min _{l} \frac{1}{\left(\Delta A_{l}\right)^{2}}, \min _{l} \frac{c_{2}^{-1} / 2}{\left(\Delta A_{l}\right)^{2}-\frac{1}{2}\left\\|\left[\sqrt{\rho}, A_{l}\right]\right\\|_{2}^{2}}\right\}\right)$ | Quantum Cramér-Rao bound |

TABLE I. Complexity of learning Hamiltonians via Gibbs states. The error $\epsilon$ is the $l_{2}$-distance error in the estimate of the Hamiltonian parameters. We use the related quantity $\epsilon_{\text {err }}$, defined via $\sum_{l=1}^{M} \operatorname{var}\left(\hat{\mu}_{l}\right)=\epsilon_{\text {err }}^{2}$. Our sample-complexity lower bound, uniquely among the approaches, (i) is based on the commutativity of the Hamiltonian's terms with the Gibbs state and (ii) requires no assumptions about the Hamiltonian's structure. In contrast, previous studies were conducted for low-interaction Hamiltonians (each term in the Hamiltonian is supported on a constant number of qubits). The question marks (?) indicate that no value has been reported or is available. Among the five prior studies, three provide no lower bounds on sample complexity. Therefore, the "key technique" is listed as NA ("not applicable") for these studies.


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