Thermal states of random quantum many-body systems

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We study a distribution of thermal states given by random Hamiltonians with a local structure. We show that the ensemble of thermal states monotonically approaches the unitarily invariant ensemble with decreasing temperature if all particles interact according to a single random interaction and achieves a state t-design at temperature $O(1/\log(t))$. For the system where the random interactions are local, we show that the ensemble achieves a state 1-design. We then provide numerical evidence indicating that the ensemble undergoes a phase transition at finite temperature.

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Introduction.— In quantum many-body systems, the number of degrees of freedom increases exponentially with the number of particles. This leads to difficulties for analysing their physics. One way to circumvent this difficulty is to assume random interactions and study typical properties of random many-body Hamiltonians, as developed in random matrix theory [1]. A study of random Hamiltonians has been extended to quantum spin systems on a lattice [2–4], where Hamiltonians should respect the local structure of the system. Such random local Hamiltonians were shown in Refs. [8–9] to have a distribution of eigenvalues different from that of random Hamiltonians without local structure, which we call random global Hamiltonians.

The idea of randomisation was also applied to a study of the typical properties of quantum states. It has been revealed that random states are almost maximally entangled [10–13], and the distribution of entanglement of random states undergoes various phase transitions [11, 16–19]. It has also been pointed out that the entanglement of random states plays a crucial role in physics from the foundation of quantum statistical mechanics [24–27] to the black hole information paradox [24–27]. Random states are also known to have a wide range of applications to quantum information processing [28–32], however, they cannot be efficiently generated if the dimension of the Hilbert space is large. Hence, an ensemble of states, called an $\epsilon$-approximate state t-design $\Upsilon^{(t)}$, that approximately simulates random states up to the order $t$ statistical moments has been studied [34–43]. An $\epsilon$-approximate state t-design is defined by $||E_{\Psi \in \Upsilon^{(t)}}[\Psi \otimes t] - E_{\Psi \in \Upsilon}[\Psi \otimes t]|| \leq \epsilon$, where $E = |\Psi \rangle \langle \Psi|$ is a density matrix for $|\Psi \rangle \in \mathcal{K}$, $E$ represents an expectation over an ensemble, and $||A||_1 = \text{tr}|A|$ is the trace norm. The expectation over random states $E_{\Psi \in \Upsilon}[\Psi \otimes t]$ is calculated to be $\Pi_{\text{sym}}^{(t)}/d_{\text{sym}}^{(t)}$ by using Schur’s lemma [44], where $\Pi_{\text{sym}}^{(t)}$ is a projection operator onto a symmetric subspace of $\mathcal{K} \otimes t$ and $d_{\text{sym}}^{(t)} = \text{tr}\Pi_{\text{sym}}^{(t)} = \binom{D+t-1}{t}$. When $\epsilon = 0$, a state t-design is called exact and we denote it simply by $\Upsilon_t$. Since a state t-design converges to random...
states when \( t \to \infty \), the distance between a given ensemble of states and a state \( t \)-design provides a measure of how uniformly the ensemble is distributed.

**Random Global and Local Hamiltonians.**— We define random Hamiltonians by using the Gaussian unitary ensemble GUE(\( L \)), which is an ensemble of \( L \times L \) Hermitian matrices \( \{ H \} \) distributed according to the Gaussian measure \( d\mu(H) \) with density proportional to \( \exp[-\frac{1}{4} \text{tr} H^2 I] \). Since it does not have any local structures, we call the GUE the ensemble of random global Hamiltonians. An important feature of random global Hamiltonians is that they are invariant under unitary conjugation, that is, \( d\mu(uHu^\dagger) = d\mu(H) \) for any \( u \in U(L) \) where \( U(L) \) is the unitary group of degree \( L \). Hence, their ground states are random states.

We also introduce the ensemble of random \( k \)-local Hamiltonians: consider a system consisting of \( n \) particles with \( k \)-body interactions, where the dimension of each particle is \( d \). We denote by \( \mathcal{H} = (C^d)\otimes^n \) the corresponding Hilbert space. The system is described by a hypergraph \( \mathcal{G} = (V, \mathcal{E}) \), where \( V(\mathcal{E}) \) is a set of vertices (hyperedges) and \( |V| = n \), and we identify each hyperedge with a \( k \)-body interaction. An ensemble of Hamiltonians \( \mathcal{H}_k \) of the form \( H = \sum_{\mathcal{E} \in \mathcal{E}} h_\mathcal{E} \) is called the ensemble of random \( k \)-local Hamiltonians when each \( h_\mathcal{E} \) is independently chosen from GUE(\( d^n \)). Note that \( \mathcal{H}_k = \text{GUE}(d^n) \) is the ensemble of random global Hamiltonians. Unlike random global Hamiltonians, random \( k \)-local Hamiltonians for \( k \neq n \) do not have global unitary invariance and their ensemble of ground states differs from the unitarily invariant one.

At finite temperature \( T \), a state of a system at thermal equilibrium is given by a thermal state \( \rho_T(\beta) := e^{-\beta H}/Z_T(\beta) \), where \( \beta = 1/T \) is the inverse temperature and \( Z_T(\beta) = \text{tr} e^{-\beta H} \) is the partition function. Although a thermal state is in general not a pure state, we straightforwardly extend the definition of a \( t \)-design to a mixed state and define a distance between an ensemble of thermal states \( \{ \rho_T(\beta) \} \) and a state \( t \)-design by \( T_t^{(k)}(\beta) := \frac{1}{2} ||E_{H \in \mathcal{H}_k}[\rho_T(\beta) - \rho_T(\beta)]\|_1 \). If an ensemble of thermal states satisfies \( T_t^{(k)}(\beta) = \epsilon/2 \) for some \( \beta \), average properties of the system can be described by an \( \epsilon \)-approximate state \( t \)-design up to order \( t \).

**Random Global Hamiltonian systems.**— We first study the ensemble of thermal states for random global Hamiltonians \( \mathcal{H}_n \). Since an ensemble of their ground states is unitarily invariant, we investigate how the ensemble converges at finite temperature to the unitarily invariant one with decreasing temperature. When \( t = 1 \), \( E_{H \in \mathcal{H}_n}[\rho_T(\beta)\otimes^n] \) reduces to the completely mixed state \( I_D/D \), where \( D = d^n \) and \( I_D \) is the identity matrix in \( \mathcal{H} \), since it commutes with all \( u \in U(D) \) due to the unitary invariance of \( \mathcal{H}_n = \text{GUE}(D) \). Hence, \( T_t^{(n)}(\beta) = 0 \) for any \( \beta \), implying that the ensemble of thermal states is a state 1-design at any temperature. For \( t \neq 1 \), we show below that the distance \( T_t^{(n)}(\beta) \) for any \( t \) monotonically decreases when \( \beta \) increases.

For the sake of simplicity, we denote \( Z_T(\beta) \) by \( X(\beta) \). Due to the unitary invariance of the GUE and the invariance of the partition function under unitary conjugation, \( X(\beta) \) commutes with any unitary matrices of the form of \( u\otimes^t \) \( (u \in U(D)) \), \( u\otimes^t X(\beta) (u\otimes^t) = X(\beta) \). From Schur-Weyl duality [1], it follows that \( X(\beta) = (\lambda\Pi_{sym}^{(\beta)}) \oplus A \), where \( \lambda = \frac{1}{d_{sym}} \text{tr} X(\beta) \Pi_{sym} < 1/d_{sym} \), and \( A \) is some operator on the space orthogonal to the symmetric subspace. Hence, we obtain \( \Pi_{sym}^{(t)} X(\beta) \Pi_{sym} = \lambda(\beta) \Pi_{sym}^{(t)} \). Recalling that \( \Pi_{sym}^{(t)} = \Pi_{sym}^{(t)}/d_{sym} \), \( T_t^{(n)}(\beta) \) is divided into two distances such as \( T_t^{(n)}(\beta) = \| \Pi_{sym}^{(t)} X(\beta) \|_{1/2} + \| \Pi_{sym}^{(t)} X(\beta) - \Pi_{sym}^{(t)}/d_{sym} \|_{1/2} \), where \( \Pi_{sym}^{(t)} \) is the identity operator on \( H^{\otimes t} \). Moreover, by using a fact that \( \lambda(\beta) \geq 1/d_{sym} \), \( T_t^{(n)}(\beta) \) is calculated to be

\[
T_t^{(n)}(\beta) = 1 - \text{tr} X(\beta) \Pi_{sym}^{(t)},
\]

To further simplify the expression, we project the operator \( \Pi_{sym}^{(t)} \) as \( \frac{1}{\lambda} \sum_{\sigma \in S_t} V_{\sigma} \), where \( S_t \) is the permutation group of order \( t \) and \( V_{\sigma} \) is a unitary representation of \( \sigma \). Using the formula that \( \text{tr} V_{\sigma} \rho^{\otimes t} \rho^{\otimes c} = \text{tr} \rho^{c} \) for a cyclic element \( \sigma \) in the permutation group, where \( |c| \) is the order of the cycle, \( T_t^{(n)}(\beta) \) is rewritten as a function of purities of thermal states as follows:

\[
T_t^{(n)}(\beta) = 1 - \frac{1}{t!} \sum_{\sigma \in S_t} \text{E}_{\mathcal{H}_n} \prod_{\sigma \in \sigma} \text{tr} (\rho_H(\beta))^{\sigma},
\]

where the product is taken over all cycles in \( \sigma \).

We finally show that \( \frac{\partial}{\partial \beta} T_t^{(n)}(\beta) < 0 \) for any \( \beta \), which implies a monotonic decrease of \( T_t^{(n)}(\beta) \) with respect to \( \beta \). It suffices from Eq. [2] to show \( \frac{\partial}{\partial \beta} \text{tr} (\rho_H(\beta)) = m \frac{Z_{H_{\beta}}(\lambda_{H_{\beta}})}{Z_{H}(\lambda_{H})} \geq 0 \) for any natural number \( m \). This simply holds since \( \frac{\partial}{\partial \beta} \text{tr} (\rho_H(\beta))^{m} = \text{tr} \sum_{m=0}^{\infty} \text{E}_{\mathcal{H}_n}[\rho_H^{(m)}(\beta)] (H_{\beta} - (H_{\beta})_{m\beta}) \), where \( (H_{\beta}) := \text{tr}[H \rho_H(\beta)] \) is an internal energy of \( H \) at the inverse temperature \( \beta \), and the internal energy satisfies that \( (H_{\beta}) \geq (H_{\beta})_{m\beta} \) for \( \beta \leq \beta' \). The equality holds if and only if \( \beta = 0, \infty \).

When \( \beta = 0 \), a thermal state \( \rho_H(\beta) \) is the completely mixed state \( I_D/D \), so that \( T_t^{(n)}(0) = 1 - d_{sym}/d^{t} \), which is approximately given by \( 1 - 1/t! \) for a constant \( t \). On the other hand, \( \lim_{\beta \to \infty} T_t^{(n)}(\beta) = 0 \) since ground states of random global Hamiltonians are random states. Hence, \( T_t^{(n)}(\beta) \) monotonically decreases from \( 1 - 1/t! \) to zero with decreasing temperature.

For sufficiently large \( t \) and \( \beta \), \( T_t^{(n)}(\beta) \) can be further calculated from Eq. [3]. Let \( H = \sum_{m=0}^{D-1} E_m = E_0 = E_1 = \ldots \) be an eigenvalue decomposition of \( H \), where the eigenvalues satisfy \( E_i \leq E_j \) for \( i < j \). Using this notation, Eq. [1] is rewritten as \( T_t^{(n)}(\beta) = \)
FIG. 1: Panel (a) shows upper bounds on $T_t^{(n)}(\beta)$ for $D = 4$, where $t = 11, 8, 5, 2$ from top to bottom. The inset shows the scaling of $T_t^{(n)}(\beta)/t$ with $\beta$ for $t = 3, 6, 9, 12$ from top to bottom, which indicates that $T_t^{(n)}(\beta)$ scales as $t e^{-c\beta}$ for large $\beta$. Panel (b) shows a sufficient temperature for thermal states of $\mathcal{H}_n$ to be an $\epsilon$-approximate $t$-design for $\epsilon = 0.5, 0.4, 0.3, 0.2$ from top to bottom.

\[1 - \operatorname{tr}\mathbb{E}_{\mathcal{H}_n} \left[ \sum_{m_1, \ldots, m_t} p_{m_1}(\beta) \otimes_{j=1}^t |E_{m_j} \rangle \langle E_{m_j} | \right] \geq 0,\]

where the summation runs over all $m_1, \ldots, m_t \in \{0, \ldots, D - 1\}$. Since $\operatorname{tr} \left[ \sum_{m_1, \ldots, m_t} |E_{m_j} \rangle \langle E_{m_j} | \right] = 1$ when $m_i = m_j$ for all $i, j \in \{1, \ldots, t\}$ and is at most $O(1/t)$ otherwise, $T_t^{(n)}(\beta)$ is simply given by

\[T_t^{(n)}(\beta) = 1 - \operatorname{tr}\mathbb{E}_{\mathcal{H}_n} \left[ \sum_{m} p_{m}(\beta) |E_{m} \rangle \langle E_{m} | \right] - O(1/t),\]

where we have used that $\operatorname{tr}\mathbb{E}_{\mathcal{H}_n} \left[ |E_{m} \rangle \langle E_{m} | \right] = (D/2)^t$ for any $n \in \{0, \ldots, D - 1\}$. Moreover, when $\beta$ is sufficiently large such that $t \beta \gg 1/D E$ where $D E = E_1 - E_0$, it is approximately given by

\[T_t^{(n)}(\beta) = 1 - \operatorname{tr}\mathbb{E}_{\mathcal{H}_n} \left[ (p_0(\beta))^t \right].\]

Note that this provides, in general, an upper bound for $T_t^{(n)}(\beta)$, and it becomes exact when $\beta \to \infty$. Since the joint probability distribution of $\{E_k\}_{k=1}^{D-1}$ for $\mathcal{H}_n$ is known [24,27], an upper bound of $T_t^{(n)}(\beta)$ can be numerically (but exactly) calculated as given in Fig. 1.

From Eq. (3), we also obtain the scaling of a threshold temperature $T_c$, below which the ensemble of thermal states is an $\epsilon$-approximate $t$-design. Since $(p_0(\beta))^t \sim 1 - t e^{-\Delta E \beta}$ for large $t$ and $\beta$, $T_t^{(n)}(\beta) \sim O(t e^{-c\beta})$, where $c$ is a constant. Thus, we obtain that $T_c = O((\log t + \log 1/\epsilon)^{-1})$. The numerics show that this holds even for relatively small $t$ (see the inset of Panel (a) and Panel (b) in Fig. 1). Thus, average properties of random global Hamiltonian systems at temperature $O((\log t + \log 1/\epsilon)^{-1})$ are describable by an $\epsilon$-approximate $t$-design. Since an $\epsilon$-approximate $t$-design for small $t$ also shares important properties of random states, such as a scrambled feature [24,27], and can be replaced with random states in many quantum informational tasks using them [48], so does the ensemble of thermal states in random global Hamiltonian systems at the corresponding temperature.

Random Local Hamiltonian systems.-- For random local Hamiltonians, the investigation of $T_t^{(k)}$ is not as simple as that for global ones since the ensemble of Hamiltonians $\mathcal{H}_n$ consisting of local terms does not, in general, have unitary invariance. However, the ensemble of thermal states of $\mathcal{H}_n$ for any $k$ is still an exact state $t$-design at any temperature, i.e. $T_t^{(k)}(\beta) = 0$, as shown below.

The $\mathcal{H}_n$ still remains invariant under the conjugation of local unitary operations of the form $\otimes_{i=1}^n u_i$, where $u_i \in U(d)$. Hence, the ensemble $\mathbb{E}_{\mathcal{H}_n}[\rho_H(\beta)]$ also commutes with all local unitary matrices, implying that it is in the commutant of them: $\mathbb{E}_{\mathcal{H}_n}[\rho_H(\beta)] = (\otimes_{i=1}^n U(d))'$, where $X'$ is the commutant of an algebra $X$. Since the commutant of the tensor products is the same as the tensor product of the commutants of each algebra, $(\otimes_{i=1}^n U(d))' = \otimes_{i=1}^n (U(d))'$, known as the commutation theorem for tensor products [44]. $\mathbb{E}_{\mathcal{H}_n}[\rho_H(\beta)]$ is in $\otimes_{i=1}^n (U(d))'$. Recalling $(U(d))' = \{I_d\}$ and $\operatorname{tr}\mathbb{E}_{\mathcal{H}_n}[\rho_H(\beta)] = 1$, we obtain $\mathbb{E}_{\mathcal{H}_n}[\rho_H(\beta)] = I_D/D$. This implies that $\mathcal{H}_n$ is an exact $t$-design for any $k$ and for any $\beta$.

We numerically study how close the ensemble of thermal states is to higher designs. We particularly consider neighboring interactions on a line of qubits. The results are given for $n = 5$ and $t = 2$ in Fig. 2. It is observed that the distance $T_2^{(k)}(\beta)$ quickly decreases with increasing $\beta$ in a small $\beta$ regime. However, when $\beta$ is larger than a certain value, $T_2^{(k)}(\beta)$ is almost constant. This limiting values depend on $k$ and are smaller for larger $k$, which is intuitively natural since the ensemble becomes random states when $k = n$ and $\beta \to \infty$. It is also observed in Fig. 2 that $T_2^{(k)}(\beta)$ monotonically decreases with $\beta$ when $k \neq 2$. In the case of $k = 2$, there exists a dip around $\beta = 1$, which is also observed for different $n$.

Panel (b) in Fig. 2 shows that the two regimes of the ensemble of thermal states, a quickly spreading regime and a converging regime, are likely to be separated by a singular point $\beta_{c}^{(k)}$. This indicates an existence of a phase transition between the two regimes. When $\beta < \beta_{c}^{(k)}$, $\partial_\beta T_2^{(k)}(\beta)$ scales quadratically with $\beta$, while
it approaches zero exponentially for $\beta > \beta_c(k)$ if $k \neq 2$.

For $k = 2$, $\partial_\beta T_t^{(k)}(\beta)$ approaches a positive value exponentially and then decreases to zero, which reflects the dip of $T_t^{(2)}(\beta)$. Although the kink of $\partial_\beta T_t^{(k)}(\beta)$ at $\beta_c(k)$ is less prominent for larger $k$, it seems present for $k = n - 1$ but not for $k = n$, where the ensemble converges slowly and smoothly to the unitarily invariant one with decreasing temperature. From these observations, we conjecture that $T_t^{(k)}(\beta)$ ($k \neq n$) has a singular point $\beta_c(k)$ in the thermodynamic limit ($n \to \infty$), leading to a second-order phase transition of the distribution of thermal states. Note that, although these results are obtained for neighboring interactions on a line, we numerically checked that most of the features are present for the case of interactions on a complete graph, except that $T_t^{(k)}(\beta)$ and $\partial_\beta T_t^{(k)}(\beta)$ do not monotonically decrease in terms of $k$ in a high-temperature region.

A possible interpretation of the distinctive temperature $\beta_c(k)$, combined with a fact that the expected density of states for the ensemble of random local Hamiltonians is a Gaussian $[6, 8]$, is that the distribution of eigenstates with low energies intrinsically differs from those with intermediate energies. To explain this clearly, let $P(E) \Delta E \propto \exp[-(E - \bar{E})^2/2\sigma^2] Z(\beta) \Delta E$ be the population between eigenstates of the energy $[E, E + \Delta E]$ for a small $\Delta E$ in a thermal state, where $\bar{E}$ and $\sigma$ is the mean and the standard deviation of the Gaussian density of states, respectively. When $\beta$ is sufficiently small such that the thermal population $e^{-\beta E}/Z(\beta)$ is close to $1/d^n$ for any $E$, the Gaussian term in $P(E)$ is dominant. Hence, the corresponding thermal state is effectively described by a mixture of the eigenstates with eigenergies in $[\bar{E} - \sigma, \bar{E} + \sigma]$. On the other hand, the thermal population in $P(E)$ becomes dominant when $\beta$ is large. For instance, the population of eigenstates with energy $E \in [\bar{E} - \sigma, \bar{E} + \sigma]$ is comparable with that of ground states at $\beta E = (E - E_0)/\sigma^2$. For $\beta \gg \beta E$, eigenstates with energy $E$ does not contribute to the thermal state any more.

Due to this trade off between the Gaussian and the thermal factors in $P(E) \Delta E$, $T_t^{(k)}(\beta)$ in a small (large) $\beta$ is expected to reflect the properties of eigenstates with intermediate (low) eigenergies. The $\beta_c(k)$ point is understood as the point where this transition happens. The singularity of $T_t^{(k)}(\beta)$ at $\beta_c(k)$ then indicates that the distribution of intermediate eigenstates for $H \in \mathfrak{S}_k$ is qualitatively different from that of low-energy eigenstates. Since $T_t^{(k)}(\beta)$ rapidly decrease with $\beta$ when $\beta < \beta_c(k)$, we also expect that the distribution of intermediate eigenstates is close to the unitarily invariant one.

The situation is entirely different for the ensemble of random global Hamiltonians for the following two reasons. First, there is no trade off between the density of states and the thermal population in $P(E)$ since the density of states obeys the semi-circle law $[1]$, which is given by $\sqrt{1 - (E - E_{\mu})^2}$. This is negligible at any temperature compared to the thermal population that exponentially scales with $E$. Second, the ensemble of eigenstates of any eigenenergy is unitarily invariant, which is in sharp contrast to the distribution of eigenstates of random local Hamiltonians, which may depend on their eigenergies. For these reasons, a distinctive temperature is not observed for the ensemble of random global Hamiltonians.

These results show that the distribution of thermal states in random $k$-local Hamiltonian systems has a rich structure and is qualitatively different from that in global Hamiltonian systems, even if $k = O(n)$. This is not only interesting from a theoretical point of view but also physically important since it means that higher-order properties in random $k$-local Hamiltonian systems cannot be inferred from random global Hamiltonian systems nor from random states even if $k = O(n)$ and the temperature is sufficiently low. Since most of the previously known results of random states related to physical situations $[20, 21]$ rely on higher-order properties, they cannot be directly applied to many-body systems where interactions are local.

**Summary and outlook.** In this Letter we have investigated a distribution of thermal states in random global/local Hamiltonian systems. For random global Hamiltonians, we analytically showed that the ensemble of thermal states monotonically approaches the unitarily invariant one with decreasing temperature and achieves an $\epsilon$-approximate state $t$-design when the temperature is $O(1/(\log t + \log 1/\epsilon))$. On the other hand, the ensemble of thermal states for random $k$-local Hamiltonians achieves a state 1-design but not higher designs. Nevertheless, we showed by numerically studying a higher design that the ensemble has a rich structure, namely, it has two regimes of temperature, a regime where the ensemble quickly spreads toward the uniform one with decreasing temperature and a regime where the ensemble converges to a non-uniform one. These two regimes are likely to be separated by a singular point, meaning that there exists a phase transition of the ensemble at finite temperature. This feature indicates an intrinsic difference of the distribution of eigenstates with intermediate energies and that with low energies.

These studies have revealed the differences and the similarities of random global/local Hamiltonians from the viewpoint of the distribution of thermal states. It is desirable to analytically confirm the features numerically observed in this paper. Proving the phase transition of the ensemble of thermal states is especially important. It is also interesting to derive the probability distribution of ground states in random local Hamiltonian systems, by which an understanding of local Hamiltonian systems will be further deepened.

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