Thermal Equilibration between Two Quantum Systems

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Two identical *finite* quantum systems prepared initially at different temperatures, isolated from the environment, and subsequently brought into contact are demonstrated to relax towards Gibbs-like quasiequilibrium states with a common temperature and small fluctuations around the time-averaged expectation values of generic observables. The temporal thermalization process proceeds via a chain of intermediate Gibbs-like states. We specify the conditions under which this scenario occurs and corroborate the quantum equilibration with two different models.

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The derivation of thermodynamic phenomena from deterministic time-reversible dynamics constitutes one of the primary goals of physics. This long-standing conundrum has sparked recently a new wave of activity in the quantum domain, where current studies of the objective follow essentially two tracks. The first one, pioneered by Schrödinger [1], leads to an understanding of canonical thermalization when the system of interest is coupled to a much larger system, a quantum giant [2–6]. The studies along the second track explore the "microcanonical" thermalization within a single isolated quantum system [7–12] and employ exact numerical diagonalization of many-body models [13,14].

Here, we focus on a different route by elucidating the process of *mutual* equilibration between two finite quantum "peers," prepared initially at different temperatures and then set into a contact. We consider two systems, A and B, that are identical, in the sense that they have identical Hamiltonians: $H_A = H_B \equiv H_S$. The Hamiltonian H_S has $\mathcal{N}_S$ nondegenerate energy levels $\{\epsilon_k\}$, $k = 1, \ldots, \mathcal{N}_S$, i.e., $H_S|\phi_k\rangle = \epsilon_k|\phi_k\rangle$, with eigenstates $\{|\phi_k\rangle\}$. The systems interact through a contact, which allows only for energy transfer without exchange of particles. The Hamiltonian of the composite bipartite system thus reads

$$H^\lambda = H_A \otimes \mathbf{1}_B + \mathbf{1}_A \otimes H_B + \lambda H^{\rm int}, \qquad (1)$$

with λ being a dimensionless coupling constant. The interaction Hamiltonian $H^{\rm int} = Y_A \otimes Y_B$, with operators $Y_A = Y_B \equiv Y$, is invariant under permutation $A \leftrightarrow B$ and does not commute with the Hamiltonian H_S [15].

We denote the energy eigenvalues and the corresponding eigenstates of the Hamiltonian H^λ by $\{E_n^\lambda\}$ and $\{|\psi_n^\lambda\rangle\}$, respectively. The quantities of interest, i.e., the energy level populations $p_k^A(t)$ and $p_k^B(t)$, can conveniently be calculated by using the product basis $|\psi^0_{n(k,j)}\rangle = |\phi_k\rangle \otimes |\phi_j\rangle$, which is also the eigenbasis of the composite system for $\lambda = 0$. We label the energies E_n^0 according to their decomposition into the sum of the single system energies: $E^0_{n(k,j)} = \epsilon_k + \epsilon_j = E_{n(j,k)}$. To shorten notations, we shall use either n or kj instead of $n(k, j)$. While combinations $k = j$ produce the nondegenerate energy levels $E^0_{kk} = 2\epsilon_k$, each two levels related by the permutation of indices $k \leftrightarrow j$, with $k \neq j$, are doubly degenerate, i.e., $E^0_{kj} = E^0_{jk}$. The transformation from the product basis $|\psi_n^0\rangle$ to the eigenbasis at a certain interaction strength $\lambda > 0$, $|\psi_n^\lambda\rangle$, is given by the matrix $\mathbf{\Lambda}$, with the elements $\Lambda_{n,m} = \langle\psi_m^0|\psi_n^\lambda\rangle$. Throughout this work we further assume for the Hamiltonian (1) with $\lambda \neq 0$ both the nondegeneracy $E_n^\lambda \neq E_m^\lambda$ for $n \neq m$ and the "nondegenerate energy gap condition" [3,5,6,10], meaning that nonzero energy differences $E_n^\lambda - E_m^\lambda$ and $E_s^\lambda - E_w^\lambda$ are not equal, apart from the trivial case $s = n$, $w = m$.

The energy level populations $p_k^{A(B)}(t)$ for system A (B) are given by the partial trace over system B (A) of the composite system density matrix $\varrho(t)$; for example, $p_k^A(t) = \sum_j \varrho_{kj,kj}(t)$, where $\varrho(t)$ is expressed in the product basis. In the case of canonical initial states, where only diagonal density matrix elements are initially nonzero, their evolution can be described by the linear map

$$\varrho_{n,n}(t) = \sum_m |U^\lambda_{n,m}(t)|^2 \varrho_{m,m}(0), \qquad (2)$$

where $U^\lambda_{n,m}(t) = \sum_l e^{-iE_l^\lambda t/\hbar}\Lambda^*_{l,n}\Lambda_{l,m}$. It is apparent that all necessary information is encoded in the energy spectrum $\{E_n^\lambda\}$ and in the transformation matrix $\mathbf{\Lambda}$.

For any choice of the system initial states $\varrho^A(0)$ and $\varrho^B(0)$, the mutual equilibration is guaranteed (in a sense detailed below) as long as the nondegenerate energy gap condition holds. Because of the parity $A \leftrightarrow B$, all eigenstates of the Hamiltonian H^λ are either symmetric, $|\psi^\lambda_{kj}\rangle = |\psi^\lambda_{jk}\rangle$, or antisymmetric, $|\psi^\lambda_{kj}\rangle = -|\psi^\lambda_{jk}\rangle$. Therefore, for every eigenstate of the composite system, expectation values for any local observable $\boldsymbol{O}$ (energy, level populations, etc.), associated with one quantum peer only, would be the same for the second peer: $O^A = O^B$. Having the total system prepared at time $t = 0$ in a product state $\varrho(0) = \varrho^A(0) \otimes \varrho^B(0)$, we turn on the interaction by setting $\lambda > 0$. Then, after some characteristic relaxation time

τ_{rel}, the system is expected to reach quasiequilibrium, where all diagonal elements of the two subsystem-reduced density matrices obey the relation $\varrho^A_{kk}(t) \simeq \varrho^B_{kk}(t)$. The respective total equilibrium system energies can be evaluated from the condition of energy conservation (assuming a diminutive interaction energy)

$$E^{A,B}_{\mathrm{eq}} \simeq [E^A(0) + E^B(0)]/2, \tag{3}$$

where $E^S = \sum_k \epsilon_k \varrho^S_{k,k}$ with $S = A$ or B. This is not a genuine equilibrium, since the populations still evolve in time [16], but their recurrences occur on time scale τ_{rec}, which is larger than any relevant time scale [12,17].

To gain an analytical insight, we start out from the limiting case in which the transformation matrix takes on a simple form: Any infinitesimally small interaction $\lambda \to 0$ will lift the twofold degeneracy $E^0_{kj} = E^0_{jk}$, yielding the pair of a symmetric and an antisymmetric eigenstates in the form $(1/\sqrt{2})(|\psi^0_{kj}\rangle \pm |\psi^0_{jk}\rangle)$, $k \neq j$. These eigenstates are nondegenerate and separated by a finite splitting. The eigenstates whose energies $E^0_{kk} = 2\epsilon_k$ were nondegenerate at $\lambda = 0$ are perturbed marginally only in this limit. By assuming this so resulting tridiagonal structure for the transformation matrix $\Lambda_{n,m}$, we find that the relaxation process leads to the arithmetic-mean quasiequilibrium state, with the corresponding populations reading [18]

$$p^{A,B}_k \simeq \tfrac{1}{2}[p^A_k(0) + p^B_k(0)]. \tag{4}$$

This tridiagonal structure is guaranteed to hold as long as each off-diagonal, nonzero matrix element of the interaction Hamiltonian $\lambda|H^{\mathrm{int}}_{n,m}|$ is smaller than the corresponding energy level difference in the composite system, $\Delta E_{n,m} = |E^0_n - E^0_m|$.

The characteristic feature of the arithmetic-mean equilibration is that two systems, when initially prepared in canonical states at different temperatures, $\varrho^S_{\mathrm{can}}(T_S) = e^{-H_S/k_{\mathcal{B}}T_S}/Z_S$, $Z_S = \mathrm{Tr}(e^{-H_S/k_{\mathcal{B}}T_S})$, with the diagonal elements

$$\varrho^S_{k,k}(T_S) \equiv p^S_k = \frac{1}{Z_S} e^{-\epsilon_k/k_{\mathcal{B}}T_S}, \tag{5}$$

where $k_{\mathcal{B}}$ is the Boltzmann constant, do relax to states with the same mean energy, but their energy level populations [Eq. (4)] are no longer Gibbs-like. In order to deviate from the limit in Eq. (4) the transformation matrix $\mathbf{\Lambda}$ needs to acquire a more complex structure. This is achieved by cranking up the interaction strength between the two systems. Provided that there occurs a sufficiently large number of nonvanishing off-diagonal elements $H^{\mathrm{int}}_{n,m}$, increasing the strength of interaction, but still remaining within the weak-coupling limit

$$\lambda(\epsilon^{\mathrm{int}}_{\mathcal{N}} - \epsilon^{\mathrm{int}}_1) \ll \epsilon_{N_S} - \epsilon_1, \tag{6}$$

wherein $\{\epsilon^{\mathrm{int}}_n\}$ is the spectrum of the interaction Hamiltonian H^{int}, then yields interaction blocks in the matrix $\Lambda_{n,m}$ larger than those 2×2 blocks. We expect that the presence of a more complex block structure ensures the evolution of canonical initial states $\varrho^A_{\mathrm{can}}(T_A)$ and $\varrho^B_{\mathrm{can}}(T_B)$ towards a common Gibbs-like equilibrium $\varrho^{A,B}(T_F)$, meaning that the corresponding diagonal elements are given by the relation (5) with the common temperature T_F. The "equilibrium" temperature T_F can be evaluated from Eq. (3), to yield with Eq. (5):

$$\sum_k \varepsilon_k \frac{e^{-(\varepsilon_k/k_{\mathcal{B}}T_F)}}{Z_F} = \frac{1}{2}\sum_k \varepsilon_k \left[\frac{e^{-(\varepsilon_k/k_{\mathcal{B}}T_A)}}{Z_A} + \frac{e^{-(\varepsilon_k/k_{\mathcal{B}}T_B)}}{Z_B}\right]. \tag{7}$$

We numerically validate our prediction by using two types of quantum models. Within the Bose-Hubbard model we consider the system consisting of $N = 5$ on-site interacting bosons on a one-dimensional lattice, with $L = 5$ sites and hard-wall boundaries. This results in $\mathcal{N}_S = \frac{(L+N-1)!}{(L-1)!N!} = 126$ energy levels in each single system and $\mathcal{N} = \mathcal{N}_S \times \mathcal{N}_S = 15\,876$ levels in the composite system [18]. Figure 1(a) depicts the setup, which assumes that the two systems overlap only by one site, where the bosons from the different confinements do interact. We also corroborated our findings with a randomly synthesized model, for which the Hamiltonian H_S and the interaction operator Y are independently sampled from a finite-dimensional Gaussian orthogonal ensemble of random matrices [18]. In contrast to the former many-body interacting boson model, where the interaction is strictly local, here the interaction is now acting globally, interweaving systems A and B.

For both models we find solutions that are based on the exact diagonalization of the corresponding bipartite Hamiltonians. Our main results are depicted in Fig. 1. Upon increasing the coupling constant λ within the weak-coupling limit [Eq. (6)], we detect a crossover from the arithmetic-mean quasiequilibrium populations [Eq. (4)] towards the canonical populations [Eq. (5)] with $T_S = T_F$.

An intriguing question is how the quantum equilibration unfolds in time. Figure 2 displays our finding that equilibration proceeds along a quasistatic pathway: The relaxation of an initial canonical state abides a sequence of time-dependent Gibbs-like states with time-dependent temperatures $T(t)$, intermediate between the initial temperature $T_{A(B)}$, to reach a common, final temperature T_F. This observed persistence of Gibbs shape is remarkable indeed. The only relevant result we could find in this context is that of thermal relaxation dynamics of a stylized model [19].

We next consider the case with an initial preparation given by pure states. Reproducibility of quantum thermal processes with a single "typical" state [20] carries importance in view of the foundations of statistical physics [7,21] and many-body quantum calculations [22]. We employ

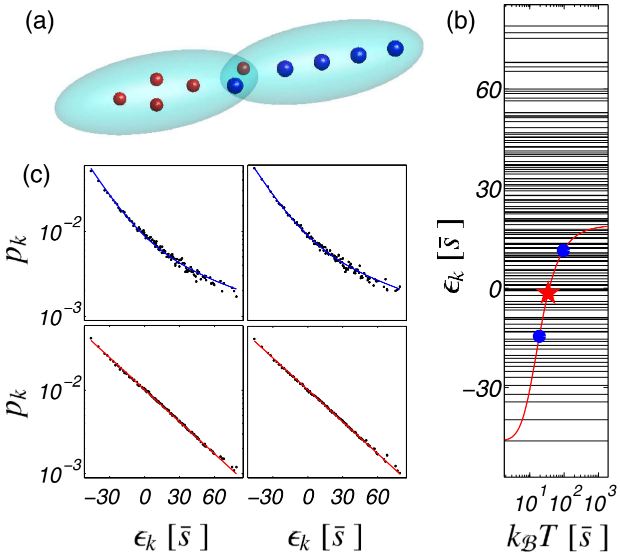

FIG. 1 (color online). (a) A system of bosons confined into two overlapping confinements is analyzed with the Bose-Hubbard model. (b) Energy spectrum of a single system. The (red) line displays the dependence of the system mean energy, i.e., $E^S = \sum_k \epsilon_k e^{-\epsilon_k/k_{\mathcal{B}}T}/Z_S$, on temperature T. The initial temperatures of the "hot" system, $k_{\mathcal{B}}T_A/\bar{s} = 94.91$, and the "cold" system, $k_{\mathcal{B}}T_B/\bar{s} = 18.98$, are indicated by the (blue) dots. The equilibrium temperature $k_{\mathcal{B}}T_F = 33.92\bar{s}$, calculated by using the total energy conservation [Eq. (7)], is indicated by the (red) star. (c) Instantaneous equilibrium energy level populations for systems A (left column) and B (right column), in the regime of arithmetic-mean (top) and thermal (bottom) equilibrations. The arithmetic-mean populations are depicted by the top (blue) solid lines, and the canonical populations for the temperature T_F by the bottom (red) lines. The natural energy unit $\bar{s}$ is given by the mean energy level spacing of the single system: $\bar{s} = (\epsilon_{\mathcal{N}_S} - \epsilon_1)/(\mathcal{N}_S - 1)$. The similar behavior is demonstrated by the second model; see supplementary material [18] for further model details.

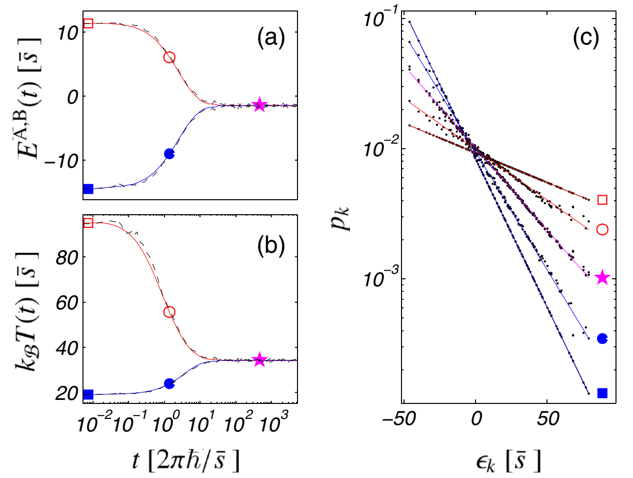

FIG. 2 (color online). Relaxation pathways for the model depicted in Fig. 1(a). Both systems are initially prepared in canonical states (solid lines) and in pure states randomly sampled from the corresponding ensembles of typical states [Eq. (8)] (dashed lines). (a) The evolution of the mean energies and (b) the corresponding temperatures $T(t)$ of the hot system A and the cold system B are shown by the upper (red) and lower (blue) lines, respectively. (c) The energy level populations of both systems are displayed at different moments of time (dots), marked by the corresponding symbols in (a) and (b). The lines correspond to the canonical populations [Eq. (5)] at the temperatures evaluated from the temporal values of mean system energies [see Fig. 1(b)].

here typical states constructed as the sums over eigenstates [20]; i.e., we use

$$|\psi^S_{T_S}(0)\rangle = \frac{1}{\sqrt{Z_S}}\sum_k e^{i\theta^S_k} e^{-\epsilon_k/2k_{\mathcal{B}}T_S}|\phi_k\rangle. \qquad (8)$$

The ensemble of typical states is defined by the uniform measure on the torus $\theta^S_1 \otimes \theta^S_2 \ldots \otimes \theta^S_N$, $\theta^S_k \in [0, 2\pi]$. The results shown in Figs. 2(a) and 2(b) by the dashed lines confirm our expectation: A single, randomly sampled, initial product wave function $|\psi^A_{T_A}(0)\rangle \otimes |\psi^B_{T_B}(0)\rangle$ follows the equilibration pathway for canonical initial states with good accuracy. Both systems A and B are prepared initially in pure states, implying vanishing von Neumann entropies $S_{A,B}(t) = -k_{\mathcal{B}}\mathrm{Tr}[\varrho^{A,B}(t)\ln\varrho^{A,B}(t)]$, i.e., $S_A(0) = S_B(0) = 0$. The isolated composite system remains in a pure state forever, and thus $S_{A\otimes B}(t) \equiv 0$. This, however, is no longer so for the subsystem entropies $S_A(t)$ and $S_B(t)$, which start to grow. From the triangle inequality it follows that $S_A(t) = S_B(t) \equiv S(t)$. The entropy $S(t)$ is a measure for entanglement between the subsystems [23]: Its monotonic growth thus indicates that the equilibration process entangles the quantum peers; see Fig. 3(a).

The systems cannot rigorously reach canonical equilibrium; therefore, the entropy $S(t)$ saturates to the value below the entropy of the Gibbs state at temperature T_F. The resulting equilibrium system density matrices $\varrho^A(t)$ and $\varrho^B(t)$ remain nonstationary and possess both diagonal and off-diagonal elements evolving in time. Following the recipe from Ref. [6], the deviation from the canonical state is estimated by using the trace-norm distance $\mathcal{D} = \mathrm{Tr}\langle|\varrho^S(t) - \bar{\varrho}^S|\rangle_t/2$, where the bar denotes the time average $\langle\ldots\rangle_t$. This quantity is limited from above [6], so that from Eq. (8) in Ref. [6] we find that $\mathcal{D} \leq 0.6$ in our case. From our numerics we obtain $\mathcal{D} \simeq 0.43$.

For an operator $\boldsymbol{O}$, which is nondiagonal in the eigenbasis of the Hamiltonian H_S, the presence of the off-diagonal elements in the system density matrices will produce additional fluctuations around the average value $\bar{O}^S = \mathrm{Tr}(\bar{\varrho}^S\boldsymbol{O})$. Moreover, some of the off-diagonal elements may possess nonzero time averages. This might cause a constant shift of the observable averaged value $\bar{O}$ from its canonical value: $\delta O^S = \bar{O}^S - \mathrm{Tr}[\bar{\varrho}^S_{\mathrm{can}}(T_F)\boldsymbol{O}]$. However, for highly nonsparse patterns of nonzero off-diagonal elements O^S_{kl} and ϱ^S_{kl}, we may expect that the respective fluctuations of the expectation value $O^S(t)$ will be suppressed, exhibiting dynamical typicality [24]. Even

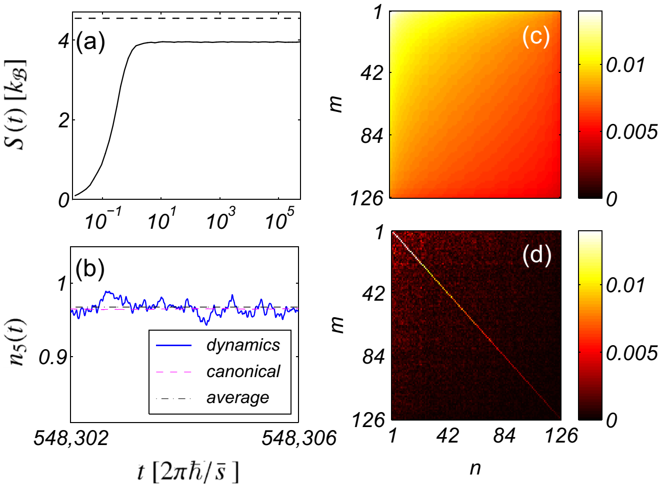

FIG. 3 (color online). (a) Von Neumann entropy of a single system vs time for the model shown in Fig. 1(a). Both systems are initially prepared in pure states randomly sampled from the ensembles of typical states [Eq. (8)]. The dashed line indicates the entropy of the Gibbs state at the temperature T_F. (b) The population dynamics $n_5(t)$ of the fifth site (i.e., the site making the thermal contact) for subsystem A is compared with the corresponding canonical value at the temperature T_F. Note that the time average of $n_5(t)$, 0.9673, differs from its canonical value, 0.9651, by 0.3% only. (c) The absolute values of reduced density matrix elements $\langle \phi_m | \varrho^A(t) | \phi_n \rangle$ at $t = 0$ and (d) after equilibration.

for a system as small as ours, with $\mathcal{N}_S = 126$ states, this mechanism works surprisingly well; see Fig. 3(b).

Thermal quantum relaxation within an isolated composite quantum system is a deterministic process and produces an output in the form of a Gibbs-like equilibrium, with diagonal elements which are almost canonical, for the initial preparation [Eq. (5)] and also for initial typical pure states [Eq. (8)]. An arbitrary choice of the initial state of the composite system H^λ does not guarantee relaxation towards Gibbs-like quasiequilibrium states for its halves. Also, the state of the composite system after relaxation is far from being Gibbs-like due to strong entanglement between its halves. Moreover, in order to render the thermodynamical relaxation of quantum peers, two necessary conditions need to be fulfilled, namely, (i) the interaction is restricted to the validity range of Eq. (6), and (ii) the total composite system obeys the parity $A \leftrightarrow B$. A natural question then is, what will happen if either of the conditions (i) or (ii) is violated? For (i) the systems will nevertheless equilibrate even with the interaction strength set beyond the weak-coupling limit. The corresponding equilibrium state, however, no longer assumes a Gibbs-like structure. The part (ii) with nonidentical systems A and B is more intricate. Although it is still possible to obtain thermal relaxation between two different systems (see [18]), the mismatch of system spectra and their relatively small sizes necessitates a much larger system-system coupling constant λ [18]. The resolution of this problem demands systems of much larger sizes and, therefore, lies outside the exact diagonalization scheme employed here.

The quasistatic character of the thermal relaxation allows for the tuning of one of the two quantum peers to a Gibbs-like state at any temperature between initial temperature values T_A and T_B, thus serving as an alternative protocol for the preparation of thermal states of quantum systems [25]. The state-of-the-art experiments with ultracold atoms provide the natural playground for exploration of the thermal relaxation between two different species of atoms [26].

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