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 quasi-equilibrium 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, 3]. The studies along the second track explore the "microcanonical" thermalization within a single isolated quantum system [4–12], 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, \( H_A = H_B = H_S \). The Hamiltonian \( H_S \) has \( N_S \) non-degenerate energy levels, \( \{ \epsilon_k \} \), \( k = 1, ..., N_S \), 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

\[
H^\lambda = H_A \otimes 1_B + 1_A \otimes H_B + \lambda H_{\text{int}},
\]

with \( \lambda \) being a dimensionless coupling constant. The interaction Hamiltonian, \( H_{\text{int}} = Y_A \otimes Y_B \), with operators \( Y_A = Y_B = Y \), 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 \( H^\lambda \) 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, \( | \psi_n^{\lambda (k,j)} \rangle = | \phi_k \rangle \otimes | \phi_j \rangle \), 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, \( E_{n(k,j)}^0 = \epsilon_k + \epsilon_j = E_{n(j,k)}^0 \). To shorten notations, we shall use either \( n \) or \( kj \) instead of \( n(k,j) \).

While combinations \( k = j \) produce the non-degenerate energy levels, \( E_{kk}^0 = 2\epsilon_k \), each two levels related by the permutation of indices \( k \leftrightarrow j \), with \( k \neq j \), are doubly degenerate; i.e., \( E_{kj}^0 = E_{jk}^0 \). 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 \( \Lambda \), with the elements \( \Lambda_{n,m} = \langle \psi_m^\lambda | \psi_n^\lambda \rangle \). Throughout this work we further assume for the Hamiltonian \( H_{\text{int}} \) with \( \lambda \neq 0 \) both the non-degeneracy, \( E_n^\lambda \neq E_m^\lambda \) for \( n \neq m \), and the "non-degenerate energy gap condition" [2, 3, 5, 6, 10], meaning that non-zero energy differences \( E_n^\lambda - E_m^\lambda \) and \( E_A^\lambda - E_B^\lambda \) are not equal, apart from the trivial case \( s = n \), \( w = m \).

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

\[
\rho_{n,n}(t) = \sum_m | \lambda_n^\lambda, \rho_{m,m}(0) = \sum_m | \lambda_n^\lambda, m,0, \]

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

For any choice of the system initial states, \( \phi^A(0) \) and \( \phi^B(0) \), the mutual equilibration is guaranteed (in a sense detailed below) as long as the non-degenerate energy gap condition holds. Due to the parity \( A \leftrightarrow B \) all eigenstates of the Hamiltonian \( H^\lambda \) are either symmetric, \( | \psi_{kj}^\lambda \rangle = | \psi_{jk}^\lambda \rangle \), or antisymmetric \( | \psi_{kj}^\lambda \rangle = -| \psi_{jk}^\lambda \rangle \). Therefore, for every eigenstate of the composite system, expectation values for any local observable \( O \) (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 \( \rho(0) = \rho^A(0) \otimes \rho^B(0) \), we turn on the interaction by setting \( \lambda > 0 \). Then, after some characteristic relaxation time \( \tau_{rel} \), the system is expected to reach quasi-equilibrium, where all diagonal elements of the two subsystem reduced density matrices obey the relation \( \rho_{kk}^A(t) \approx \rho_{kk}^B(t) \) [16]. The respective total equilibrium
system energies can be evaluated from the condition of energy conservation (assuming a diminutive interaction energy),

$$E_{eq}^{A,B} \simeq \frac{1}{2}[E^A(0) + E^B(0)],$$

(3)

where $E^S = \sum_k \epsilon_k \theta_{k,k}^S$ with $S = A$ or $B$. This is not a genuine equilibrium, since the populations still evolve in time [17], but their recurrences occur on time scale $\tau_{rec}$ which is larger than any relevant time scale [12] [18].

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 two-fold degeneracy, $E_{kj} = E_{jk}$, yielding the pair of a symmetric and an antisymmetric eigenstates in the form $\frac{1}{\sqrt{2}} \left( |\psi_{kj}^0\rangle \pm |\psi_{jk}^0\rangle \right)$, $k \neq j$. These eigenstates are non-degenerate and separated by a finite splitting.

The eigenstates whose energies, $E_{kk} = 2\epsilon_k$, were non-degenerate 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 quasi-equilibrium state, with the corresponding populations reading [19]

$$p_{k}^{A,B} \simeq \frac{1}{2} \left[ p_k^A(0) + p_k^B(0) \right].$$

(4)

This tridiagonal structure is guaranteed to hold as long as each off-diagonal, non-zero matrix element of the interaction Hamiltonian, $\lambda |H_{n,m}^{int}|$, is smaller than the corresponding energy level difference in the composite system, $\Delta E_{n,m} = |E_{n}^0 - E_{m}^0|$. The characteristic feature of the arithmetic-mean equilibrium is that two systems, when initially prepared in canonical states at different temperatures, $\theta_{can}^S(T_S) = e^{-\epsilon_k/k_BT_S}/Z_S$, $Z_S = \text{Tr}(e^{-H_S/k_BT_S})$, with the diagonal elements

$$\theta_{k,k}^S(T_S) = \frac{1}{Z_S} e^{-\epsilon_k/k_BT_S},$$

(5)

where $k_B$ 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 $\Lambda$ needs to acquire a more complex structure. This is achieved by crank up the interaction strength between the two systems. Provided that there occurs a sufficiently large number of non-vanishing off-diagonal elements, $H_{n,m}^{int}$, increasing the strength of interaction, but still remaining within the weak coupling limit

$$\lambda(\epsilon_n^{\text{int}} - \epsilon_1^{\text{int}}) \ll \epsilon_{N_S} - \epsilon_1,$$

(6)

wherein $\{\epsilon_n^{\text{int}}\}$ is the spectrum of the interaction Hamiltonian $H_{n,m}^{int}$, then yields interaction blocks in the matrix $\Lambda_{n,m}$ larger than those $2 \times 2$ blocks. We expect that the presence of a more complex block structure ensures the evolution of canonical initial states, $\theta_{can}^A(T_A)$ and $\theta_{can}^B(T_B)$, towards a common Gibbs-like equilibrium $\theta^{A,B}(T_F)$, 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):

$$\sum_k \frac{\epsilon_k}{Z_F} = \frac{1}{2} \sum_k \epsilon_k \left[ \frac{e^{-\epsilon_k/k_BT_A}}{Z_A} + \frac{e^{-\epsilon_k/k_BT_B}}{Z_B} \right].$$

(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 $N_S = \frac{L}{2} = 25$ energy levels in each single system, and $N = N_S \times N_S = 15,876$ levels in the composite system [19]. 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 (GOE) of random matrices [19]. In contrast to the former many-body interacting boson model, where the bosons from the different confinements do interact, here the interaction is strictly local.

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 $\lambda$ within the weak coupling limit, Eq. (4), we detect a crossover from the arithmetic-mean quasi-equilibrium populations, Eq. (4), towards the canonical populations, Eq. (6) 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 [20].

We next consider the case with an initial preparation given by pure states. Reproducibility of quantum thermal processes with a single ‘typical’ state [21] carries importance in view of the foundations of statistical physics [7, 22] and many-body quantum calculations [23]. We employ here typical states constructed as the sums over eigenstates [21]; i.e., we use

$$|\psi_{S}^{A}(0)\rangle = \frac{1}{\sqrt{Z_{S}}} \sum_{k} e^{i\theta_{k}^{S}} e^{-\epsilon_{k}/2k_{B}T_{F}} |\phi_{k}\rangle. \quad (8)$$

The ensemble of typical states is defined by the uniform measure on the torus $\theta_{1}^{S} \otimes \theta_{2}^{S} \cdots \otimes \theta_{N}^{S}, \theta_{k}^{S} \in [0, 2\pi]$. The results shown in Fig. 2(a, b) by the dashed lines confirm our expectation: A single, randomly sampled, initial product wave function $|\psi_{T_{A}}^{A}(0)\rangle \otimes |\psi_{T_{B}}^{B}(0)\rangle$ 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 $S_{A,B}(t) = -k_{B}T \ln \rho_{A,B}^{A}(t)$, 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 subsystem entropies $S_{A}(t)$ and $S_{B}(t)$, which start to grow. From the triangle inequality it follows that $S_A(t) + S_B(t) \geq S(t)$. The entropy $S(t)$ is a measure for entanglement between the subsystems [24]: its monotonic growth thus indicates that the equilibration process entangles the quan-

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**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. (6) (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, b). The lines correspond to the canonical populations, Eq. (6), at the temperatures evaluated from the temporal values of mean system energies (see Fig. 1(b)).

**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. (6). The dashed line indicates the entropy of the Gibbs state at the temperature $T_F$. (b) The population dynamics $n_S(t)$ of the fifth-site (i.e., the site making the thermal contact) for the subsystem $A$ is compared with the corresponding canonical value at the temperature $T_F$. Note that the time average of $n_S(t)$, 0.9673, differs from its canonical value, 0.9651, by 0.3% only. (c) The absolute values of reduced density matrix elements $\langle \phi_m | \rho | \phi_n \rangle$ at $t = 0$, and (d) after equilibration.
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, $\varrho^S(t)$ and $\varrho^D(t)$, remain nonstationary and possess both diagonal and off-diagonal elements evolving in time. Following the recipe from Ref. [3], the deviation from the canonical state is estimated by using the trace-norm distance $D = \text{Tr}[ (\varrho^S(t) - \bar{\varrho}^S) ] / 2$, where the bar denotes the time average $\langle \ldots \rangle_t$. This quantity is limited from above [3], so that from Eq. (8) in [3] we find that $D \leq 0.6$ in our case. From our numerics we obtain $D \approx 0.43$.

For an operator $O$, which is non-diagonal 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 $\bar{O}^S = \text{Tr}(\varrho^S O)$. Moreover, some of the off-diagonal elements may possess non-zero time averages. This might cause a constant shift of the observable averaged value $\bar{O}$ from its canonical value, $\delta O^S = \bar{O}^S - \text{Tr}[\varrho^S_{\text{can}}(T_F) O]$. However for highly non-sparse patterns of non-zero off-diagonal elements $O^R_{kl}$ and $g_{kl}$, we may expect that the respective fluctuations of the expectation value $O^S(t)$ will be suppressed, exhibiting dynamical typicality [25]. Even for a system as small as ours, with $N_S = 126$ 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 $H^S$ does not guarantee relaxation towards Gibbs-like quasi-equilibrium 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. (5), 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 non-identical systems $A$ and $B$ is more intricate. Although it is still possible to obtain thermal relaxation between two different systems (see [19]), the mismatch of system spectra and their relatively small sizes necessitates a much larger system-system coupling constant $\lambda^A$. 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 [20]. 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 [27].

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ARITHMETIC-MEAN EQUILIBRATION

The arithmetic-mean equilibration occurs in the limit of weak coupling between the systems, \( \lambda \{H^{\text{int}}\} \ll \{\Delta E\} \), where the transformation matrix \( \Lambda_{n,m} = \langle \psi_n^\lambda | \psi_m^\lambda \rangle \) effectively takes on the tridiagonal form, see Fig. (1a), with non-zero entries:

\[
\Lambda_{n(k,j),m(k',j')} = \begin{cases} 
1, & j = j' = k = k' \\
\frac{1}{\sqrt{2}}, & j = j' \neq k = k' \\
\chi_{kj}/\sqrt{2}, & j = j' \neq k = k', 
\end{cases} 
\]

where \( \chi_{kj} = \text{sgn}(k-j) \). Hence the dynamics of the composite system is governed by the tridiagonal evolution operator:

\[
U_{n(k,j),m(k',j')}(t) = \sum_m e^{-iE^\lambda_{m}t/\hbar} \Lambda^*_m,n \Lambda_{m,n'} 
\]

\[
= \begin{cases} 
1, & j = j' = k = k' \\
e^{i\Omega_{kj}^\lambda/2} \cos \left( \frac{\omega_{kj}^\lambda t}{2} \right), & j = j' \neq k = k' \\
e^{i\Omega_{kj}^\lambda/2} \chi_{kj} \sin \left( \frac{\omega_{kj}^\lambda t}{2} \right), & j \neq k, j' \neq k = j', 
\end{cases} 
\]

where \( \Omega_{kj}^\lambda = (E_{kj}^\lambda + E_{kj}^\lambda)/2\hbar \) and \( \omega_{kj}^\lambda = (E_{kj}^\lambda - E_{kj}^\lambda)/\hbar \). For the density matrix of the composite system written in the product basis, \( \langle \psi_n^0(k,j) | \rho | \psi_m^0(k,j') \rangle \), knowledge of its diagonal elements is sufficient for calculations of the energy level populations. For example, for the system \( A \) one has

\[
p_k^A(t) = \sum_{j=1}^{\Omega(n(k,j),n(k,j))} \theta_{n(k,j),n(k,j)}(t). 
\]

Evolution of initially diagonal states

For the systems whose initial density matrices are diagonal in \( \{|\phi^0_n\rangle\} \), \( \rho^{A,B}(0)_{k,k'} = \delta_{k,k'}p^A_{k,0} \delta_{k,B}(0) \), the evolution of the diagonal matrix elements for the composite system density matrix, \( p_n(t) = \theta_{n,n}(t) \), reduces to the linear map: \( p_n(t) = \sum_{n'} \| U_{n,n'}(t) \|^2 p_{n'}(0) \). By using the evolution operator, Eq. (2), we obtain

\[
p_{kj}(t) = \frac{1}{2} \left( p_{kj}(0) + p_{jk}(0) \right) 
+ \frac{1}{2} \cos \left( \omega_{kj}^\lambda t \right) \left( p_{kj}(0) - p_{jk}(0) \right). 
\]

The energy level populations of one system, e.g. the system \( A \) are

\[
p_k^A(t) = \frac{1}{2} \left[ p_k^A(0) + p_k^B(0) \right] 
+ \frac{1}{2} \sum_j X_{kj}^A \cos \left( \omega_{kj}^\lambda t \right), 
\]

where \( X_{kj}^A = p_k^A(0)p_j^B(0) - p_j^A(0)p_k^B(0) \).

In order to gain some physical insight it is useful to explore the following situations: (i) one of the two systems, for an example system \( B \), is initially localized on a single level, i.e. \( p_k^B = \delta_{k,B} \), and (ii) both the systems, \( A \) and \( B \), are initially localized on single levels, i.e. \( p_k^A = \delta_{k,k_A} \) and \( p_k^B = \delta_{k,k_B} \).

In the first case (i), Eq. (5) reduces to

\[
p_k^A(t) = \frac{1}{2} \left( p_k^A(0) + 1 - \sum_{j \neq k} p_j^A(0) \cos(\omega_{kj}^\lambda t), \right) k = k_B; 
\]

while for the energy level populations of the system \( B \) we obtain,

\[
p_k^B(t) = \frac{1}{2} \left( 1 + p_k^A(0) + \sum_{j \neq k} p_j^A(0) \cos(\omega_{kj}^\lambda t), \right) \right. 
\]

Thus the evolution of the energy levels with the same index \( k \neq k_B \) in the system \( A \) and the system \( B \) oscillate coherently, while the populations of energy levels with \( k = k_B \) quasiperiodically fluctuate, for all \( k \) around the arithmetic-mean of the initial populations.

In the second case (ii), the energy level populations of systems \( A \) and \( B \) read:

\[
p_k^A(t) \]

\[
= \frac{1}{2} \left\{ \begin{array}{c} 1 + 0 \cos(\omega_{kj}^\lambda t), \ k = k_A; \\ 0 + 1 \ - \cos(\omega_{kj}^\lambda t), \ k = k_B; \\
0 + 0, \ k = k_A, k = k_B; 
\end{array} \right. 
\]

and

\[
p_k^B(t) \]

\[
= \frac{1}{2} \left\{ \begin{array}{c} 0 + 1 \ - \cos(\omega_{kj}^\lambda t), \ k = k_A; \\ 1 + 0 \ + \cos(\omega_{kj}^\lambda t), \ k = k_B; \\
0 + 0, \ k = k_A, k = k_B. 
\end{array} \right. 
\]

Thus, for \( k_A \neq k_B \) each system performs coherent Rabi type oscillations between the levels \( k_A \) and \( k_B \) around
the arithmetic-mean of their initial values, while the rest of the levels remains unpopulated. Evidently, if \( k_A = k_B = k_S \) then the corresponding frequency \( \omega_{kj} \equiv 0 \), thus both systems stay localized forever and there is no dynamics at all.

**Evolution of initially pure states**

When initially both the systems are assumed to be in pure states, \( |\psi^{A,B}(0)\rangle = \sum_k \epsilon_k^{A,B} |\phi_k\rangle \) and the initial state of the composite system is given by their product, \( |\psi(0)\rangle = |\psi^{A}(0)\rangle \otimes |\psi^{B}(0)\rangle \), so that

\[
|\psi(0)\rangle = \sum_n c_n(k,j) |\psi_n(k,j)\rangle, \quad c_n = c_k^{A} c_j^{B}. \tag{6}
\]

the diagonal matrix elements of the total density matrix are

\[
p_{kj}(t) = |\langle \psi_{kj}^0 | \psi(t) \rangle|^2 = |\langle \psi_{kj}^0 | U^A(t) | \psi(0) \rangle|^2. \tag{7}
\]

Using \( c_{kj} = \sqrt{p_k^A p_j^B} \exp \left[ i(\theta_k^A + \theta_j^B) \right] \), where \( \theta_k^A (\theta_j^B) \), the phase entering the initial state of the system \( A (B) \) (see Eq. (8), of main manuscript), we end up with the the energy level populations of the system \( A \):

\[
p_k^A(t) = \frac{1}{2} \left[ p_k^A(0) + p_k^B(0) \right] + \frac{1}{2} \sum_j X_{kj}^A \cos \left( \omega_{kj}^A t \right) + \frac{1}{2} \sum_j Y_{kj}^A \sin \left( \theta_{kj} - \theta_{jk} \right) \sin \left( \omega_{kj}^A t \right), \tag{8}
\]

where \( Y_{kj}^A = \chi_{jk} \sqrt{p_k^A(0) p_j^B(0) p_j^A(0) p_k^B(0)}/2 \) and \( \theta_{kj} = \theta_k^A + \theta_j^B \). The only difference from the Eq. (5) is the last sum on the rhs. The latter is generated by non-zero off-diagonal elements of initial density matrix, \( \varrho(0) = |\psi(0)\langle \psi(0)| \).

Apparently, the evolution for diagonal initial states can also be obtained from Eq. (5) by averaging over the ensemble of pure states with the different initial phases, \( \theta_{kj} \), and fixed initial populations of the energy levels, \( p_k^{A,B}(0) \). This would lead to the nullification of the last sum on the rhs of Eq. (5).

**Relaxation to the arithmetic-mean of the initial populations**

In most physical situations, the initial energy level populations, \( p_k^{A,B}(0) \), exhibit a smooth dependence on \( k \), thus producing a significant number of non-zero coefficients \( X_{kj}^{A,B} \). This is also the case for the canonical states with \( k_B T \gg \bar{s} \), where \( \bar{s} \) denotes the mean level spacing, \( s = \left( \epsilon_{N_S} - \epsilon_1 \right)/(N_S - 1) \). The relation (5) yields \( p_k^A(0) \) at \( t = 0 \). In the course of time every member of the sum on the rhs of Eq. (5) begins acquiring a certain phase. Since the frequencies \( \omega_{kj}^A \) do not commensurate in general, after the characteristic time, \( \tau_{rel} \sim 2\pi/\omega_{ij}^{A,B} \), where \( \omega_{ij}^{A,B} \) is the root mean square of the set \( \{ \omega_{kj}^A \} \), we will obtain a sum of independent random values, almost uniformly distributed over the interval \([-1, 1]\), and weighted with the coefficients \( X_{kj}^A \). Given the initial states with a substantial number of populated energy levels, the sum looses its initial coherence completely after the time \( \tau_{rel} \) and averages itself to zero. Hence the relaxation process leads to the arithmetic-mean equilibration,

\[
p_k^{A,B} \simeq \frac{1}{2} \left[ p_k^A(0) + p_k^B(0) \right]. \tag{9}
\]

The rhs of Eq. (5) is a quasiperiodic function \( \bar{s} \), therefore it will repeat itself after some time \( \tau_{rec} \) with any given accuracy \( \Delta \), so that \( \| p_k^A(0 + T(\Delta)) - p_k^A(0) \| \leq \Delta \). Assuming, for example, that the coefficients \( X_{kj}^{A,B} \) are equal, the recurrence time grows exponentially with \( N_S \):
\[ \tau_{rec} \sim \frac{1}{N_L^2} \Gamma(N_S + 1)(\Delta N_S/4\pi)^{-(N_S-1)/2} \] 

Already for \( N_S = 10 \) and \( \Delta = 0.1 \) we find a sharp scale separation between the recurrence and relaxation times, \( \tau_{rec}/\tau_{rel} \simeq 3 \cdot 10^6 \).

**BLOCKS IN THE TRANSFORMATION MATRIX \( \Lambda \) AS INITIATORS OF THERMAL EQUILIBRATION**

Let us denote by \( |\psi_{A,s,a}^\lambda \rangle \) the pair, the symmetric and the antisymmetric eigenstates, and by \( |\psi_{A,B}^{0,0} \rangle \) their two-fold degenerate parental eigenstates, correspondingly. Here index \( A \) stands for the product state, \( |\psi_{A,B}^{0} \rangle = |\phi_b \rangle \otimes |\phi_a \rangle \), whereof the larger part of the energy, \( E_A^{0} = \epsilon_k^A + \epsilon_l^B \), is located in the system \( A \), i.e. \( \epsilon_A^A = \epsilon_k, \epsilon_B^A = \epsilon_l, \epsilon_k > \epsilon_l \). The eigenstate \( |\psi_{B}^{0} \rangle \) is given by the permutation, \( |\phi_l \rangle \otimes |\phi_k \rangle \).

In the limit of the arithmetic-mean equilibration the tridiagonal structure of the transformation matrix allows for energy exchange between levels with the same energies, \( \epsilon_A^A = \epsilon_B^B \), only. A strengthening of the interaction violates this ‘level-to-level’ rule, so that more than two eigenstates of the composite system can exchange their energies. Yet the interaction of any strength preserves the permutation symmetry. Therefore, a step beyond the arithmetic-mean equilibration consists in inclusion of a ‘coupling’ between the pair of states \( |\psi_{A,s,a}^\lambda \rangle \) and its neighbor (closest in total energy) pair, \( |\tilde{\psi}_{s,a}^\lambda \rangle \). In terms of the transformation matrix elements the coupling means that the pair \( |\psi_{A,B}^{0,0} \rangle \) contributes to the states \( |\tilde{\psi}_{s,a}^\lambda \rangle \), and the pair \( |\tilde{\psi}_{A,B}^\lambda \rangle \) contributes to the states \( |\psi_{s,a}^\lambda \rangle \). The block corresponding to this unitary transformation has the following form

\[ \left( \begin{array}{c} |\psi_{A}^\lambda \rangle \\ |\tilde{\psi}_{A}^\lambda \rangle \\ |\psi_{s,a}^\lambda \rangle \\ |\tilde{\psi}_{s,a}^\lambda \rangle \end{array} \right) = \left( \begin{array}{cccc} a & a & b & b \\ c & -c & d & -d \\ e & e & f & f \\ g & -g & h & -h \end{array} \right) \left( \begin{array}{c} |\psi_{A}^{0} \rangle \\ |\tilde{\psi}_{A}^{0} \rangle \\ |\psi_{s,a}^{0} \rangle \\ |\tilde{\psi}_{s,a}^{0} \rangle \end{array} \right). \] (10)

Assuming that only one 4×4 block is present in the transformation matrix, after tracing over one system and neglecting the oscillating elements we obtain the following ‘equilibrium’ populations of the energy levels:

\[
\begin{align*}
\rho_1^A &= \rho_1^B = \frac{1}{2} \left[ p_1^A(0) + p_1^B(0) \right] - \delta P, \\
\rho_2^A &= \rho_2^B = \frac{1}{2} \left[ p_2^A(0) + p_2^B(0) \right] - \delta P, \\
\rho_3^A &= \rho_3^B = \frac{1}{2} \left[ p_3^A(0) + p_3^B(0) \right] + \delta P, \\
\rho_4^A &= \rho_4^B = \frac{1}{2} \left[ p_4^A(0) + p_4^B(0) \right] + \delta P,
\end{align*}
\] (11)

where \( \delta P = \alpha (p_1^A(0) p_2^B(0) + p_2^A(0) p_3^B(0) - p_3^A(0) p_4^B(0) - p_4^A(0) p_1^B(0)) \). The only parameter is \( \alpha = a^4 + c^4 + e^4 + g^4 - 1/2 = b^4 + d^4 + f^4 + h^4 - 1/2, -1/2 < \alpha < 0 \). Therefore, the 4×4 block produces the unidirectional energy exchange between the pairs \( |\psi_{A\_s,a}^\lambda \rangle \) and \( |\tilde{\psi}_{s,a}^\lambda \rangle \).

The above result can be generalized to the case of a \( 2M \times 2M \) block, which involves the energy exchange between \( M \) pairs of eigenstates. The energy exchange is then parameterized by \( K \) parameters \( \alpha_{kq}, \) \( q = 1, \ldots, K \), where \( K \) is given by the number of ways to choose a pair from \( M \) elements, i.e. \( K = M(M-1)/2 \).

When the transformation matrix has a multiple-block structure, a given single system eigenstate \( |\phi_k \rangle \) may enter several blocks. Then the quasi-equilibrium energy level population for the state \( |\phi_k \rangle \) is given by

\[
\rho_k^{A,B} \simeq \frac{1}{2} \left[ p_k^A(0) + p_k^B(0) \right] + \sum_{\{sk\}}^{K_s} \sum_{q=1}^{K_k} \Phi_{kl,k_s} a_{s,k}^{a_k} a_{s,k}^{q},
\] (12)

where the sum index, \( s \), runs over the numbers of those blocks \( \{sk\} \) that the \( k \)-th state participates in, \( K_s = \frac{M_s(M_s-1)}{2} \) is the number of parameters \( a_{s,k}^{a_k} \) in the \( s \)-th block of size \( 2M_s \times 2M_s \), \( k_s \) is the index of a partner state for the \( s \)-th block, and \( k_s k_q \) denotes the product state which exchanges the energy with the product state \( k_s k \).

The typical multi-block structure of the transformation matrix \( \Lambda \) is depicted in Fig. 4(b).

To demonstrate that even a small number of \( 2M \times 2M \) blocks with \( M > 1 \) in the transformation matrix \( \Lambda \), ensures that the energy level populations, Eq. (12), approach the Gibbs-like equilibrium, we use a simple model system with \( N_S = 6 \) energy levels. We take the transformation matrix with the structure displayed in Fig. 4(c).

According to (12), the latter is fully described by the seven parameters: \( \alpha_1^1 \) (1st 2×2 block), \( \alpha_1^2 \) (2nd 2×2 block), \( \alpha_3^1 \) (3rd 2×2 block), \( \alpha_2^1 \) (4th 2×2 block) and \( \alpha_5^1 \) (5th 2×2 block). In the following, we rename, for simplicity, these seven parameters again to \( \alpha_i, i = 1, \ldots, 7 \).

The \( N \times N \) matrix, with \( N = N_S \times N_S = 36 \) entries, describes the composite system. The seven corresponding ‘exchange’ terms, \( \Phi \), composed according to Eq. (12), have the following forms:

\[
\begin{align*}
\alpha_1, \Phi_{14,23} &= p_1^1(0) p_2^4(0) + p_4^1(0) p_1^4(0) - p_2^4(0) p_3^3(0) - p_3^3(0) p_2^4(0), \\
\alpha_2, \Phi_{15,24} &= p_1^4(0) p_2^5(0) + p_5^4(0) p_1^5(0) - p_2^5(0) p_3^6(0) - p_3^6(0) p_2^5(0), \\
\alpha_3, \Phi_{16,25} &= p_1^5(0) p_2^6(0) + p_6^5(0) p_1^6(0) - p_2^6(0) p_3^5(0) - p_3^5(0) p_2^6(0), \\
\alpha_4, \Phi_{16,34} &= p_1^6(0) p_2^5(0) + p_5^6(0) p_1^5(0) - p_2^5(0) p_3^4(0) - p_3^4(0) p_2^5(0), \\
\alpha_5, \Phi_{25,34} &= p_2^5(0) p_3^4(0) + p_4^5(0) p_2^4(0) - p_3^4(0) p_5^5(0) - p_5^5(0) p_3^4(0), \\
\alpha_6, \Phi_{26,35} &= p_2^4(0) p_3^5(0) + p_5^4(0) p_2^5(0) - p_3^5(0) p_6^4(0) - p_6^4(0) p_3^5(0), \\
\alpha_7, \Phi_{36,45} &= p_3^4(0) p_6^5(0) + p_6^4(0) p_3^5(0) - p_4^5(0) p_6^5(0) - p_6^5(0) p_4^5(0).
\end{align*}
\]
The color diagram displays the root mean square deviations of block parameters, so the energy level populations, together with the arithmetic-mean of initial populations (blue lines). The three subplots (●, ♦, ⭐) show the energy level populations (dots) in linear-log scale, for the three different sets of values of block parameters, $\alpha_1 = \alpha_j = j = 2, \ldots, 7$, indicated by the corresponding symbols on the color diagram. In addition, the canonical populations (straight red lines) is plotted together with the arithmetic-mean of initial populations (blue lines).

So the energy level populations, $p_k^{A,B}(0), k = 1, \ldots, 6$, approach and fluctuate around the equilibrium populations $p_k^{A,B}$:

$$p_1^{A,B} = p_1^{ar} + \alpha_1 \Phi_{14,23} + \alpha_2 \Phi_{15,24} + \alpha_3 \Phi_{16,25} + \alpha_4 \Phi_{16,34},$$

$$p_2^{A,B} = p_2^{ar} - \alpha_1 \Phi_{14,23} - \alpha_2 \Phi_{15,24} - \alpha_3 \Phi_{16,25} + \alpha_4 \Phi_{16,34},$$

$$p_3^{A,B} = p_3^{ar} - \alpha_1 \Phi_{14,23} + \alpha_4 \Phi_{16,34} - \alpha_5 \Phi_{25,34},$$

$$p_4^{A,B} = p_4^{ar} + \alpha_1 \Phi_{14,23} - \alpha_2 \Phi_{15,24} + \alpha_3 \Phi_{16,25} - \alpha_5 \Phi_{25,34} + \alpha_7 \Phi_{36,45},$$

$$p_5^{A,B} = p_5^{ar} + \alpha_2 \Phi_{15,24} - \alpha_3 \Phi_{16,25} + \alpha_5 \Phi_{25,34} - \alpha_6 \Phi_{26,35} - \alpha_7 \Phi_{36,45},$$

$$p_6^{A,B} = p_6^{ar} + \alpha_3 \Phi_{16,25} + \alpha_4 \Phi_{16,34} + \alpha_6 \Phi_{26,35} + \alpha_7 \Phi_{36,45},$$

where $p_k^{ar} = (p_k^A + p_k^B)/2$ denote the arithmetic-mean.

Figure 2 displays the above equilibrium populations of the six energy levels, $\epsilon_k, k = 1, \ldots, 6$, possessed by the system of two bosons in three-site lattice, with the initial temperatures $k_B T_A = (\epsilon_2 - \epsilon_1)/2$, $k_B T_B = \epsilon_6 - \epsilon_1$. To measure the deviation from the canonical population, we calculate the root mean square deviation (RMSD) of the populations $p_k^A$ from the canonical populations at the temperature $T_F$, evaluated from the condition of energy conservation, Eq. (7) of the main manuscript:

$$\Delta(\alpha_1, \alpha_2, \ldots, \alpha_7) = \sqrt{\sum_{k=1}^{6} [p_k^A - p_k(T_F)]^2} / 6.$$
normal distribution with dispersion \( \sigma \), set to one in dimensionless units. It has been rescaled to the mean level spacing \( \bar{s} \), so that \( \sigma = 3.55\bar{s} \). The constraint on the Hamiltonian, \([H_S]_{n,n'} = [H_S]_{n',n}, n, n' = 1, \ldots, N\), provides its hermiticity. The interaction Hamiltonian, \( H^{\text{int}} \), was modelled by the direct product of two identical random matrices from GOE, generated independently, by using the same procedure. The parameters used in calculations are: \( \lambda U^{\text{int}} = 2.72 \cdot 10^{-4} \bar{s} \) (the arithmetic-mean equilibration, Fig. 3(c), top) and \( \lambda U^{\text{int}} = 5.45 \cdot 10^{-3} \bar{s} \) (the thermal equilibration, Fig. 3(c), bottom), \( k_B T_A = 1363.81 \bar{s} \), \( k_B T_B = 34.09 \bar{s} \), \( k_B T_F = 81.05 \bar{s} \).

CROSSOVER FROM THE ARITHMETIC-MEAN TO THE THERMAL EQUILIBRATION

In this section we provide the details of the crossover between the regimes of ‘arithmetic-mean’ and thermal equilibrations. We analyze the state of the subsystem \( A \) represented by its energy level populations \( p_k^A(t) \), after the relaxation from initial Gibbs state. To quantify the deviation of the actual ‘equilibrium’ state from the arithmetic-mean or Gibbs-like states, we employ the distance between energy level populations:

\[
D^{\text{ar,can}}_p = \sum_k |p_k^{\text{ar,can}} - \langle p_k^A \rangle_t| \tag{16}
\]

where \( \langle \ldots \rangle_t \) denotes the time-average evaluated after the equilibration, \( \tau_{\text{rec}} > t > \tau_{\text{rel}} \), and \( p_k^{\text{ar}} (p_k^{\text{can}}) \) are the populations of the corresponding arithmetic-mean (Gibbs-like) state.

Figure 4 shows the results of the calculations for the bosonic model, Eq. (14), with three different sets of the particle numbers, \( N \), and the lattice sizes, \( L \): \( (N, L) = (4, 4), (4, 5), (5, 5) \), which result in the Hilbert spaces of size, \( N_S = 35, 70, 126 \), respectively. The other parameters of the corresponding Hamiltonians are the same as in the previous section, i.e. \( J/U = 7/3 \), \( k_B T_A = 5(U + J) \), and \( k_B T_B = U + J \).

The numerical results demonstrate the presence of a smooth crossover between the arithmetic-mean and thermal regimes of equilibration. The regimes reveal themselves by the plateau-like minima of \( D^{\text{ar,can}}_p \). The increase of system size \( N_S \) sharpens the crossover, note the log-scale in Fig. 4. In addition, there are three notable features: (i) the crossover region shifts to the region of smaller coupling strengths, thus squeezing the
FIG. 5: The same distances as in Fig. 4 but as functions of the coupling strength rescaled by the mean level spacing of the corresponding system. After the scaling, in contrast to Fig. 4, the systems of different size share the same crossover region (open circle). Note, that due to the logarithmic scale of $x$-axis, the region of the thermal equilibration is much broader than that of the arithmetic-mean equilibration.

The results of the scaling depicted in Figure 5 support this hypothesis. The inset of Fig. 4 shows that the mean energy level spacing scales like $N_S^\xi$, with the exponent $\xi \sim -0.8$. This also provides us with the scaling of the arithmetic-mean region with increasing of the system size. The scaling exponent seems to depend on the mean lattice occupation number $\langle n \rangle$ and the ratio of the Hamiltonian parameters, $J/U$, only.

DIFFERENT SYSTEMS IN CONTACT

Here we present the example of the equilibration process between two quantum systems with different spectra and initial temperatures, but the same size of the Hilbert space, $N_A = N_B$, see Fig. 6. The lack of the permutation symmetry, $A \leftrightarrow B$, leads to the absence of two-fold degeneracies in the composite system at $\lambda = 0$, meaning that an infinitesimal coupling strength $\lambda > 0$ does not modify significantly the spectrum of composite system any more, in contrast to the previous case of two identical systems in contact. Therefore different subsystems do not exhibit the regime of arithmetic-mean equilibration. At very weak coupling, which would induce the arithmetic-mean equilibration for two identical systems, the ‘thermal equilibration’ between different systems occurs locally, i.e. within a number of independent clusters of energy levels only. In order to render the thermal equilibration process between the subsystems of rather small sizes, $N_A = N_B = 126$, we had to choose a relatively large value of the coupling constant, which is close to the upper bound of the weak coupling limit, Eq. (6) of main manuscript.
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