Tuning canonical typicality by quantum chaos

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One key issue of the foundation of statistical mechanics is the emergence of equilibrium ensembles in isolated and closed quantum systems. Recently, it was predicted that in the thermodynamic ($N \to \infty$) limit the canonical density matrix emerges for small subsystems from almost all pure states of large quantum many-body systems. This notion of “canonical typicality” is assumed to originate from the entanglement between subsystem and environment and the resulting intrinsic quantum complexity of the many-body state. We show that quantum chaos plays a crucial role in the emergence of canonical typicality for large but finite quantum systems. We demonstrate that the degree of canonical typicality can be quantitatively controlled and tuned by the degree of quantum chaoticity present in the many-body system.

I. INTRODUCTION

As first recognized by Ludwig Boltzmann [1, 2] “molecular” chaos lies at the core of the foundation of classical statistical mechanics. Only when the phase space of an isolated mechanical system is structureless can the motion be assumed to be ergodic and the equal-a priori probability for phase space points on the energy hyper-surface is realized. This is the basic tenet of the microcanonical ensemble. Moreover, chaotic dynamics is “mixing” thereby enforcing the approach to the thermal equilibrium state from “almost all” out-of-equilibrium initial conditions. In turn, any well-defined small subsystem that is only allowed to exchange energy with the remainder of the large isolated system described by the microcanonical ensemble (referred to as bath or environment in the following) is described by the canonical ensemble. The phase-space density of the subsystem is weighted by the Boltzmann factor $e^{-\beta H_s}$ where $H_s$ is the Hamilton function of the subsystem, $\beta = 1/k_B T$ with $T$ the temperature imprinted by the environment and $k_B$ the Boltzmann constant. However, when the phase space of the system is not chaotic but rather dominated by regular motion on KAM tori [3, 4], neither ergodicity nor mixing is assured and thermalization of an initial non-equilibrium state may be elusive. The implicit assumption of classical equilibrium statistical mechanics is that in the limit of a large number of degrees of freedom chaos is generic for any interacting many-particle system.

How those concepts translate into quantum physics has remained a topic of great conceptual interest and lively debate [5–10]. Renewed interest is stimulated by the experimental accessibility of ultracold quantum gases [11–14] and nano-systems [15, 16] where many of the underlying concepts became quantitatively accessible in large but finite quantum systems in unprecedented detail. The foundation of thermalization of quantum systems has been pioneered by von Neumann in term of the quantum ergodic theorem [17–22]. Accordingly, the entropy is an increasing function of time and expectation values of generic macroscopic observables for pure states formed by coherent superposition of states within microscopic energy shells converge to that of the microcanonical ensemble provided that the energy spectrum of the system is strictly non-degenerate. Recently, this description of thermal equilibrium states was extended to the notion of “canonical typicality” [22–25]. Accordingly, starting from almost any pure state from the microcanonical ensemble of the large isolated many-body system, the reduction to a small subsystem by tracing out the degrees of freedom of the bath will yield the canonical density matrix $\hat{\rho}_s = e^{-\beta H_s} / \text{Tr}[e^{-\beta H_s}]$ with $H_s$ the Hamilton operator of the subsystem. The proof of this canonical typicality invokes the intrinsic randomness of the expansion coefficients of the pure state in terms of entangled subsystem-bath states. This assumption goes back to the notion of intrinsic quantum complexity of entangled states in large systems put forward already by Schrödinger [26].

An alternative approach to thermalization is tied to the eigenstate thermalization hypothesis (ETH) [5–8] based on the notion of quantum chaos. Specific signatures characterizing quantum chaos were originally identified in few-degrees of freedom systems whose classical limit exhibits chaos [27–30]. Nowadays, the notion of quantum chaos is invoked for systems that display the same signatures such as energy level distributions predicted by random matrix theory (RMT) [27, 31, 32] or randomness of wavefunction amplitudes [5] even when a well-defined classically chaotic counterpart does not exist. The ETH conjectures that the diagonal matrix elements of any generic local observable taken in the energy eigenstate basis are smooth functions of the total energy while the off-diagonal elements are exponentially decreasing randomly fluctuating variables with zero mean [6–8]. The ETH has been shown to hold for a large variety of systems without a classical analogue [11, 33–43]. Deviations from the ETH have been observed in finite Fermi-Hubbard and Bose-Hubbard systems [37, 38, 44] when the energy level

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distribution deviates from the Wigner-Dyson level statistics of RMT characteristic for chaotic systems.

In the present paper we explore the quantitative relationship between canonical typicality and quantum chaos. More specifically, we want to address the widely open question: What happens to canonical typicality in the transition between integrable and chaotic dynamics? Is quantum chaos a condition sine qua non for the emergence of the Gibbs ensemble (canonical ensemble) or is quantum entanglement and complexity in these systems itself sufficient to render the reduced density operator of a small subsystem canonical? We explore this connection by exact diagonalization of a large yet finite quantum system. As a prototypical case in point we consider an impurity embedded in a spin-polarized Fermi-Hubbard system. In this system the impurity can serve as a “thermometer” in the isolated many-body quantum system providing an unambiguous subsystem-bath decomposition with tunable coupling strength between subsystem and bath. Moreover, this system features a tunable transition from quantum chaos to quantum integrability. We measure the proximity of the reduced density matrix of the impurity to the canonical density matrix and identify a strong and direct correlation between the degree of canonical typicality and of quantum chaos.

The paper is structured as follows. In Sec. II we introduce our impurity-Fermi-Hubbard model which serves as a prototypical (sub)system-environment model system. The mapping of spectral properties of this isolated many-body system onto thermal states of the impurity within the framework of the microcanonical and canonical ensembles are discussed in Sec. III. The distance in Liouville space between the reduced density matrix of the impurity and a generic canonical density matrix is analyzed in Sec. IV and the relation between the degree of canonical typicality and quantum chaos is established. Concluding remarks are given in Sec. V.

II. THE FERMI-HUBBARD MODEL WITH IMPURITY

We investigate a variant of the single-band one-dimensional Fermi-Hubbard model which is particularly well suited to study entanglement and quantum correlations between subsystem and its environment or bath. The bath is represented by spin-polarized fermions enforcing single occupancy of sites by bath particles while the distinguishable impurity can occupy any site. Accordingly, the Hamiltonian of the total system is given by

\[ \hat{H} = \hat{H}_I + \hat{H}_B + \hat{H}_{IB}, \]

where the Hamiltonian of the subsystem, i.e. the impurity (I), is

\[ \hat{H}_I = -J_I \sum_{j=1}^{M_s-1} [\hat{a}_{j+1}^\dagger \hat{a}_j + c.c.] + \sum_{j=1}^{M_s} V(j) \hat{n}_j, \]

while the Hamiltonian of the bath is

\[ \hat{H}_B = -J_B \sum_{j=1}^{M_B-1} [\hat{b}_{j+1}^\dagger \hat{b}_j + c.c.] + \sum_{j=1}^{M_B} \tilde{V}(j) \tilde{n}_j, \]

and the interaction between the subsystem and the bath is given by

\[ \hat{H}_{IB} = W_{IB} \sum_{j=1}^{M_s} \tilde{n}_j \tilde{n}_j. \]

The operators \( \hat{a}_j \) and \( \hat{a}_j^\dagger \) (\( \hat{b}_j \) and \( \hat{b}_j^\dagger \)) are the creation and annihilation operators of the impurity (bath particles) on site \( j \), and \( \tilde{n}_j = \hat{a}_j^\dagger \hat{a}_j \) (\( \tilde{N}_j = \hat{b}_j^\dagger \hat{b}_j \)) the corresponding number operators. \( J_I \) (\( J_B \)) describes the hopping matrix elements of the impurity (bath particles). The bath particles interact with each other by a nearest-neighbor interaction with strength \( W_{BB} \) while the impurity interacts with the bath particles via an on-site interaction with strength \( W_{IB} \). The Hubbard chain has \( M_s \) sites with Dirichlet boundary conditions imposed at the edges. An additional very weak external background potential \( (V \ll J_I, J_B) \) with on-site matrix element \( V(j) \) (\( j = 1, \ldots, M_s \)) is applied,

\[ V(j) = 0.01 \left[ -0.5 + \frac{(j-1)^n}{(M_s - 1)^n} \right], \]

for which we use a linear (\( n = 1 \)) or quadratic (\( n = 2 \)) function removing residual geometric symmetries such that the irreducible state space coincides with the entire state space and symmetry related degeneracies are lifted.

We solve the system via exact diagonalization to determine all eigenstates and eigenenergies of the system. The dimension of the Hilbert space of the entire system is \( d_H = s_{s^2}^{M_s N_B} \), where \( N_B \) is the number of bath particles. We consider typical half-filling configurations with \( N_B \approx M_s/2 \). The largest \( M_s \) considered is \( M_s = 15 \) resulting in a Hilbert space dimension of \( d_H = 96525 \) for \( N_B = 7 \). We set \( J_I = J_B = J \) which also defines the unit of energy (\( J = 1 \)) in the following. We consider both a weak (\( W_{IB} \ll 1 \)) and a moderate subsystem-bath coupling (\( W_{IB} = 1 \)) to explore its role in establishing a thermal state. The key advantage of the present model is that it allows to control and tune the properties of the bath separately by varying \( W_{BB} \) while keeping fixed the properties of the subsystem whose reduced density matrix we probe. This unique subsystem-bath decomposition allows for the unambiguous probing of canonical typicality thereby avoiding any ad-hoc separation by “cutting out” of the subsystem which then requires the grand canonical density matrix for such an open quantum system [44]. The present single-band Fermi-Hubbard model does...
not possess an obvious classical counterpart whose phase space consists of regions of regular and/or chaotic motion. Lacking such direct quantum-classical correspondence, quantum integrability and quantum chaos in the present system will be identified by those measures of the spectrum of the quantum system that have been shown to signify chaotic and regular motion in systems where quantum-classical correspondence does prevail. As will be shown below, by tuning $W_{BB}$ we can continuously tune the entire system, from the limit of quantum integrability to the limit of quantum chaos across the transition region of a mixed quantum phase space in which integrable and chaotic motion coexist and explore its impact on canonical typicality.

Starting point for analyzing quantum chaos by means of level statistics is the cumulative spectral function also called the spectral staircase function

$$N(E) = \sum_{\alpha} \Theta(E - E_{\alpha}),$$

where $E_{\alpha}$ are the energy eigenvalues of the entire system, and $\Theta$ is the Heaviside step function. Its spectral derivative is the density of states (DOS)

$$\Omega(E) = \frac{d}{dE} N(E).$$

Examples for $N(E)$ and $\Omega(E)$ are shown in Fig. 1. The smoothed “average” spectral staircase function $\bar{N}(E)$ fitted to a polynomial of order 10, also shown in Fig. 1, provides the reference for spectral unfolding required for certain measures of quantum fluctuations about the (classical) mean. Accordingly, the unfolded energy spectrum is given by $e_{\alpha} = \bar{N}(E_{\alpha})$. For systems for which quantum-classical correspondence holds, $\bar{N}(E)$ would correspond to the classical phase space volume in units of Planck’s constant $h$ and $\Omega(E)$ [Fig. 1 (b)] to the microcanonical energy shell. The saturation of $N(E)$ with increasing $E$ [Fig. 1 (a)] or, likewise, the bell-shaped curve for the DOS [Fig. 1 (b)] is specific to single-band models with a finite bandwidth and is not present in a generic many-particle system.

The probability density $P(s)$ of the nearest-neighbor level spacings (NNLS), $s = e_{\alpha+1} - e_{\alpha}$, features distinctively different shapes for quantum integrable and quantum chaotic systems. While for integrable systems the NNLS has been predicted by Berry and Tabor [31] to feature a Poissonian distribution $P_P(s) = \exp(-s)$, for chaotic systems it closely follows random matrix theory [27]. In our case of a time-reversal symmetric system the corresponding random-matrix ensemble is the Gaussian orthogonal ensemble (GOE) which has been shown (see e.g. [28]) to closely follow the Wigner-Dyson distribution (or Wigner surmise) given by

$$P_{WD}(s) = \frac{\pi s}{2} e^{-\pi s^2/4}.$$  (8)

The search for a generic NNLS distribution in the regime of a mixed phase space in which integrable and chaotic motion coexist has remained an open problem. For systems with a classical counterpart several models have been proposed [45–49]. Empirically, the best fit to spectral data for mixed systems has been provided by a heuristic ansatz suggested by Brody [50] which allows for a one-parameter smooth interpolation of the NNLS distribution between the quantum integrable and quantum chaotic limit,

$$P_B(s) = (\gamma + 1) b s^\gamma e^{-bs^{\gamma+1}}$$  (9)

with

$$b = \left[ \Gamma \left( \frac{\gamma + 2}{\gamma + 1} \right) \right]^{\gamma+1},$$  (10)

where the Brody parameter $\gamma$ varies between $\gamma = 0$ (integrable) to $\gamma = 1$ (chaotic). The parametrization of this transition in term of a variable exponent $\gamma$ has the salient feature that even for very small but finite $\gamma$, $0 < \gamma < 1$, $P_B(0) = 0$, i.e. even any weak perturbation of quantum integrability immediately suppresses the probability density for any exact degeneracy. Non-degeneracy is one of the key requisites of von Neumann’s quantum ergodic theorem [17]. For mixed few-degrees of freedom systems
with a classical analogue, $\gamma$ has been found to be a measure for the chaotic fraction of phase space [48, 51]. To determine $\gamma$ we alternatively fit Eq. 9 either directly to the data for $P(s)$ or to its integral $\int_0^s ds' P(s')$. Differences provide an error estimate for the fit [Fig. 2 (c)]. As the intra-bath interaction is varied from $W_{BB} = 0.01$ to $W_{BB} = 1$ we observe a transition from a near Poissonian to an approximate Wigner-Dyson NNLS distribution [Fig. 2 (a), (b)]. For any $W_{BB} > 0$, all degeneracies are removed and $P(s = 0) = 0$. The Brody parameter monotonically increases from $\gamma \simeq 0.05$ at $W_{BB} = 0.01$ to $\gamma \simeq 0.9$ at $W_{BB} = 1$. We note that after reaching a plateau at $\gamma \simeq 0.93$ near $W_{BB} = 3$, the Brody parameter decreases again for $W_{BB} > 5$ and vanishes in the strongly correlated limit of $W_{BB} \gg 1$. The value of $W_{BB}$ where the plateau region is reached agrees well with the critical parameter for which the Mott metal-insulator transition has been observed in the Fermi-Hubbard system [52]. The decrease of the Brody parameter results from clustering of the energy spectrum in the strongly interacting regime into separate regions. The bath fragments into clusters of particles with the interactions between separate clusters suppressed. Thus, a partially ordered system emerges reducing the quantum chaoti
city. We will focus in the following on the parameter range $W_{BB} \leq 1$.

We note that recently a complementary measure of the chaoti
city in the level statistics has been proposed [53, 54] that has the advantage that it does not require spectral unfolding but can be applied to the spectral raw data. The distribution $W(r)$ of restricted gap ratios $r_{\alpha}$

$$
W(r) = \frac{2}{(1 + r)^2}.
$$

The present Fermi-Hubbard systems obeys these predictions for both the quantum integrable ($W_{BB} \rightarrow 0$) and near quantum chaotic limit ($W_{BB} \gtrsim 0.9$) very well (Fig. 3) confirming that the identification of integrability and chaos is independent of the particular choice of spectral measure. For the first moment of the restricted gap ratio distribution we find $\langle r \rangle = 0.5284$ for $W_{BB} = 1$ close to the GOE expectation value for asymptotically large matrices $\langle r \rangle_{GOE} = 0.5307$ [54]. Conversely, for $W_{BB} = 0$ we find $\langle r \rangle = 0.3826$ in very good agreement with the prediction for a Poisson distribution $\langle r \rangle_P = 0.3863$. As there is presently no interpolation function $W(r)$ for the transition between the quantum integrable limit (Eq. 13) and the quantum chaotic limit (Eq. 12) available, we will focus in the following on the Brody distribution for the NNLS.

We will consider the regime $0 < W_{BB} \leq 1$ in which the system can be continuously and monotonically tuned from quantum integrability to quantum chaos. The dependence of the Brody parameter $\gamma$ on the interaction parameter of the bath particles, $\gamma(W_{BB})$, [Fig. 2 (c)] can be remarkably accurately approximated by the function $\gamma(W_{BB}) \approx \gamma_0 \tanh(W_{BB}/W_{BB}^0)$ ($\gamma_0 = 0.88, W_{BB}^0 = 0.15$).

III. THE REDUCED DENSITY MATRIX OF THE IMPURITY

The impurity embedded in the Fermi-Hubbard system serves as a “thermometer”, i.e. as a sensitive probe of the thermal state of the interacting many-body system. We aim at exploring the emergence of the mixed state for the impurity when the entire (subsystem and bath)
The system is in a pure and stationary eigenstate of $\hat{H}$ with vanishing von Neumann entropy $S_{vN} = 0$ and energy $E_\alpha$. We then pose the following question: Starting from a given isolated eigenstate of the entire system, under which conditions will the reduced density matrix of the impurity correspond to a canonical density matrix, i.e. the thermometer will be in a Gibbs state? And if such a thermal state emerges, what will be its temperature $T$, or its inverse temperature $\beta = 1/k_B T$? We refer to this process as emergence of a thermal equilibrium state rather than the frequently used term “thermalization” as the latter (implicitly) implies a time-dependent approach to an equilibrium state starting from an out-of-equilibrium (mixed or pure) initial state. We neither invoke any ensemble average over states from the microcanonical energy shell of finite thickness $\Delta E$ nor do we invoke wave packet dynamics of a non-stationary state of the entire system.

According to standard equilibrium statistical mechanics for closed systems, the inverse temperature of subsystems is controlled by the density of states $\Omega_B(E)$ of the bath at the most probable energy sharing between subsystem and bath. Accordingly, the bath imprints the inverse temperature

$$\beta(E) = \frac{\partial \ln \Omega_B(E)}{\partial E}$$

on the subsystem, i.e. the impurity. As the density of states of the impurity $\Omega_\alpha(E - E_B)$ is small compared to that of the bath, the DOS $\Omega_B(E)$ of the bath in Eq. 14 can be well approximated by that of the entire system

$$\beta(E) = \frac{\partial \ln \Omega(E)}{\partial E},$$

which establishes a direct connection between inverse temperature and the DOS extracted from exact diagonalization (Fig. 1). In the thermodynamic limit Eq. 14 and Eq. 15 would be strictly equivalent. For a finite quantum system, they are only approximately equal and Eq. 15 will feature smaller fluctuations because of the increased ensemble size.

Exploring the ensemble equivalence in the thermodynamic limit we can alternatively determine an implicit relation between $\beta$ and $E$ through the canonical expectation value applied to the entire system

$$E = \frac{\text{Tr} \left[ \hat{H} e^{-\beta \hat{H}} \right]}{\text{Tr} \left[ e^{-\beta \hat{H}} \right]} = \frac{\partial \ln Z_c}{\partial \beta},$$

where $Z_c = \text{Tr} \left[ \exp \left(-\beta \hat{H} \right) \right]$ is the canonical partition function and $\hat{H}$ is the Hamiltonian of the entire system (see Eq. 1). Again, in the thermodynamic limit Eq. 15 and Eq. 16 should yield equivalent results for $\beta(E)$. Our finite system appears to be large enough such that discrepancies between the microcanonical and canonical description are small. The dependence of the inverse temperature on the energy of the entire system derived either from the microcanonical (Eq. 15) or canonical relation (Eq. 16) is shown in Fig. 4 for the case of the moderately strong bath-bath interaction $W_{BB} = 1$. In spite of the fact that the size of our system is far from the thermodynamic limit ($N \to \infty$), the agreement between the two
thermodynamic ensembles is already remarkably close. Deviations are mostly noticeable in the region of negative $\beta$ where the DOS decreases rather than increases with $E$ which is a peculiarity of the single-band model. The density operator of the entire system in any pure energy eigenstate $|\psi_\alpha\rangle$ is given by the projector $|\psi_\alpha\rangle\langle\psi_\alpha|$. Consequently, the reduced density matrix (RDM) of the impurity follows from tracing out all bath degrees of freedom,

$$D^{(I)}_\alpha = \text{Tr}_B [|\Psi_\alpha\rangle\langle\Psi_\alpha|],$$

which will, in general, depend on the parent state $|\psi_\alpha\rangle$ it is derived from. We explore the canonical typicality of $D^{(I)}_\alpha$ emerging from each individual eigenstate $|\psi_\alpha\rangle$ of the entire system, by diagonalizing $D^{(I)}_\alpha$

$$D^{(I)}_\alpha = \sum_{j=1}^{M_\alpha} n_{j,\alpha} |n_{j,\alpha}\rangle\langle n_{j,\alpha}|,$$

yielding natural occupation numbers $n_{j,\alpha}$ and natural orbitals $|n_{j,\alpha}\rangle$. Ideally, $n_{j,\alpha}$ should be given by the Boltzmann factor $e^{-\beta \epsilon^{(I)}_{j,\alpha}}$ with $\epsilon^{(I)}_{j,\alpha}$ the expectation value of the Hamilton operator of the impurity evaluated in the basis of natural orbitals, $\epsilon^{(I)}_{j,\alpha} = \langle n_{j,\alpha}|H_I|n_{j,\alpha}\rangle$, which, in turn, should be close to the eigenstates of $H_I$. Moreover, the $\beta$ in the Boltzmann factor should coincide with that extracted from the bath using either the microcanonical (Eq. 15) or canonical approach (Eq. 16) and should be independent of $\alpha$. For a system with a finite impurity-bath coupling, the residual interaction with the bath needs to be taken into account on the mean-field (MF) level

$$\epsilon^{(I)}_{j,\alpha} = \langle n_{j,\alpha}|(H_I + \hat{W}^{(IB)}_{\text{MF},\alpha})|n_{j,\alpha}\rangle,$$

where the MF interaction operator in site-basis reads

$$W^{(IB)}_{\text{MF},\alpha}(m) = W_B \rho_{B,\alpha}(m)$$

and

$$\rho_{B,\alpha}(m) = |\langle m|\psi^{(B)}_\alpha\rangle|^2$$

is the density of bath particles in state $|\psi_\alpha\rangle$ projected onto the site $m$. The energy fluctuations

$$\Delta \epsilon^{(I)}_{j,\alpha} = \sqrt{\langle n_{j,\alpha}|(H_I + \hat{W}^{(IB)}_{\text{MF},\alpha})^2|n_{j,\alpha}\rangle - \epsilon^{(I)}_{j,\alpha}^2}$$

provide a measure of the proximity of the natural orbitals of the RDM to the eigenstates of the (perturbed) Hamilton operator of the subsystem. It should be noted that in the limit of very weak impurity-bath coupling these MF corrections will become negligible. An example for the natural-orbital occupation number distribution of the impurity RDM emerging from a single energy eigenstate of the entire system with state index $\alpha = 4364$ (with $\alpha$ sorted by energy) and energy eigenvalue $E_\alpha = -2.396$ lying on the tail of the DOS with positive $\beta$ for $W_{BB} = 1$ is shown in Fig. 5. Indeed, the Boltzmann distribution $\propto e^{-\beta \epsilon^{(I)}_{j,\alpha}}$ characterizing the canonical density matrix is observed. Moreover, the fit to an exponential with $\beta = 0.58$ predicted by the microcanonical ensemble for the entire system (Eq. 15) reproduces the distribution of occupation numbers very well. Thus, the emergence of a canonical density matrix from the reduction of state $\alpha = 4364$ is verified.

**IV. CANONICAL TYPICALITY AND BRODY PARAMETER**

The demonstration of the emergence of the canonical density matrix from a particular eigenstate $|\psi_\alpha\rangle$ of the entire system invites now the crucial question: Will this (almost) always work as implied by the notion of canonical typicality? Is this a generic feature of the complexity of entangled quantum states in large systems or does this require, in analogy to classical statistical mechanics, specific dynamical properties of the underlying system? We explore these questions by investigating the behavior of $\beta$ as a function of the exact total energy $E_\alpha$ for the complete set of states $\alpha$ of the entire system and for two different values of the bath-bath interaction, $W_{BB} = 1$ in the quantum chaotic regime with Brody parameter $\gamma \approx 0.9$ [see Fig. 2 (b)] and $W_{BB} = 0.1$ in the mixed quantum integrable-chaotic regime with $\gamma = 0.5$ [see Fig. 2 (c)].

Striking differences appear (Fig. 6): While for chaotic dynamics in the bath a thermal distribution with a well-defined temperature, consistent with the (mi-
of $\Delta \beta$ for each value $W$.

The approach of the RDM of the impurity to the (ideal) Gibbs state
$$D_{\alpha}^{Gibbs} = \frac{1}{Z_{c,\alpha}} e^{-\beta_{\alpha} (\hat{H}_I + \hat{W}_{MF,\alpha})},$$
with
$$Z_{c,\alpha} = \text{Tr}[e^{-\beta_{\alpha} (\hat{H}_I + \hat{W}_{MF,\alpha})}]$$
can be directly observed in the site representation $(m_1, m_2)$ of the RDM [Fig. 8 (b)]. We illustrate the site representation of the RDM for two energetically nearest-neighbor states ($\alpha = 13637$ and $\alpha = 13678$) in the mixed region ($W_{BB} = 0.1$). We quantify the approach to the Gibbs state through the density matrix site correlation function
$$C_{\alpha}(\Delta m) = \sum_{m=1}^{M} D_{\alpha}^{(1)}(m, m + \Delta m).$$

While the state $\alpha = 13638$ results in a nearly diagonal RDM in the site basis [Fig. 8 (a)] with rapidly decaying site correlations closely following the prediction by the Gibbs state (Eq. 22), the adjacent state $\alpha = 13637$ yields an RDM with significant off-diagonal entries, extended site correlations, and strong deviations from the

FIG. 6. The parameter $\beta$ as a function of energy $E_\alpha$ for each eigenstate of the entire system obtained from fits to the RDM of the impurity as in Fig. 5 for two different bath-bath interaction strengths $W_{BB}$, (a) $W_{BB} = 1$ with $\gamma \approx 0.9$ and (b) $W_{BB} = 0.1$ with $\gamma \approx 0.5$. The color code represents the variance of $\beta_\alpha$ obtained from the fit and is chosen such that all variances above $\Delta \beta_\alpha > 0.01$ are plotted as red. The lines correspond to $\beta(E)$ obtained from the microcanonical ensemble Eq. 15 (solid) and the canonical ensemble Eq. 16 (dashed), respectively. Other parameters in both (a) and (b) are $M_s = 15$, $N_B = 7$, and $W_{IB} = 1$.

FIG. 7. The fraction of canonical density matrices $G$ obtained for the RDM of the impurity as a function of the Brody parameter $\gamma$. The dots are color-coded by the interaction strength $W_{BB}$ between the bath particles. The error bar on the x-axis corresponds to the error bar of the Brody parameter as in Fig. 2 (c), while the error bar on the y-axis is determined by calculating the mean and standard deviation of the fraction resulting from different thresholds of $\Delta \beta_{th}$. The straight line corresponds to $G(\gamma) = \gamma$. Other parameters are $M_s = 15$, $N_B = 7$, and $W_{IB} = 1$.

up to $\Delta \beta_{th} = 1.5 \times 10^{-2}$. The emerging trend (Fig. 7) is, however, unaffected by the particular choice of $\Delta \beta_{th}$. The uncertainty in the threshold directly enters the error bars. The fraction of canonical density matrices representing a Gibbs state, $G(\gamma)$, monotonically increases with quantum chaoticity as parametrized by the Brody parameter $\gamma$ which, in turn, monotonically increases with the bath interaction $W_{BB}$. The approach of the RDM of the impurity to the (ideal) Gibbs state

$G_{\alpha}^{Gibbs} = \frac{1}{Z_{c,\alpha}} e^{-\beta_{\alpha} (\hat{H}_I + \hat{W}_{MF,\alpha})}$,

with
$Z_{c,\alpha} = \text{Tr}[e^{-\beta_{\alpha} (\hat{H}_I + \hat{W}_{MF,\alpha})}]$ can be directly observed in the site representation $(m_1, m_2)$ of the RDM [Fig. 8 (b)]. We illustrate the site representation of the RDM for two energetically nearest-neighbor states ($\alpha = 13637$ and $\alpha = 13678$) in the mixed region ($W_{BB} = 0.1$). We quantify the approach to the Gibbs state through the density matrix site correlation function

$C_{\alpha}(\Delta m) = \sum_{m=1}^{M} D_{\alpha}^{(1)}(m, m + \Delta m)$. (23)
the dependence of $\gamma$ on $\gamma'$ with $\gamma'$ being much larger.

Overall, we can provide preliminary evidence to this effect by exploring the scaling with system size still within computational reach. The degree of quantum chaoticity as measured by the Brody parameter $\gamma$, indeed, increases with system size at fixed strength of the interaction $W_{BB}$ that breaks quantum integrability (Fig. 9). We vary the system size by increasing the total number of sites while keeping the system at (approximate) half-filling of bath particles. The corresponding Hilbert space increases from $d_H = 22308$ ($M_s = 13, N_B = 6$) to $d_H = 96525$ ($M_s = 15, N_B = 7$). The observed increase of quantum chaoticity with system size is qualitatively in line with properties of classical chaos: In a mixed phase space with locally surviving tori their influence on phase space dynamics is rapidly diminishing with increasing phase space dimensions a prominent example of which is Arnold diffusion [3, 4]. This increase of quantum chaoticity with system size at fixed interaction strength turns out to be key for the emergence of the interrelation between the degree of canonical typicality and quantum chaos as both the Brody parameter $\gamma$ as well as the fraction of density matrices complying with the Gibbs state increases with system size at fixed bath interaction strength. As a consequence a near universal relation $G(\gamma)$ between the fraction of (approximate) Gibbs states and the degree of quantum chaos as measured by $\gamma$ emerges (Fig. 10). The data for different combinations of values of $W_{BB}$ and $M_s$ fall on the same curve. Overall, the dependence of $G$ on $\gamma$ can be very well approximated by a function $G(\gamma) \approx \tanh^{2}(\gamma/\gamma_0)$ with $\gamma_0 = 0.46$.

We have thus established that the degree of canonical
FIG. 10. Universal relation between the fraction $G$ of RDMs of the impurity converging to a Gibbs state and the Brody parameter $\gamma$ for different combinations of systems size ($M_s$ and $N_B$) and bath interaction strengths $W_{BB}$. The gray straight line corresponds to a linear increase of $G(\gamma) = \gamma$, while the black curve shows a fit to $G(\gamma) = \tanh^2(\gamma/\gamma_0')$ with $\gamma_0' = 0.46$. Impurity-bath interaction in all systems $W_{IB} = 1$.

typicality, i.e. the likelihood that a subsystem is in a Gibbs state when the large system it is embedded in is in a pure energy eigenstate with zero von Neumann entropy is controlled and can be tuned by the degree of level repulsion in the quantum many-body system. The latter can be viewed as a direct signature of chaotic quantum dynamics.

V. CONCLUSIONS AND OUTLOOK

In this work we have explored the emergence of a thermal (Gibbs) equilibrium state of a small (sub)system in thermal contact with a bath when the combined large but finite quantum system is isolated and in a well-defined energy eigenstate. As prototypical case we have considered an impurity embedded in an interacting spin-polarized Fermi-Hubbard many-body bath which facilitates a clear-cut subsystem-bath decomposition and a tunable transition of the entire system from quantum integrability to quantum chaos. We have shown that quantum chaos is the essential prerequisite for “canonical typicality” of almost all stationary energy eigenstates of the entire system, i.e. the emergence of a canonical density matrix for the reduced density matrix of the impurity by tracing out bath degrees of freedom. Each of these eigenstates represents the fine-grained version of the energy shell of the microcanonical ensemble of the impurity-bath system. Quantum chaos, identified here by an energy-level statistics in accord with the Wigner-Dyson surmise of random matrix theory, is shown to play a key role in establishing a Gibbs state of the subsystem in direct analogy to the role of classical chaos which Boltzmann invoked in deducing the classical (micro-)canonical ensemble. One can thus view this as an extension of classical-quantum correspondence to this cornerstone of the foundation of statistical mechanics.

For the finite quantum system we could identify a continuous transition from the emergence of a thermal state to its breakdown controlled by the degree of quantum chaoticity as parametrized by the Brody parameter of level statistics. Even though our simulations are limited to finite-size systems, the present results for varying system sizes suggest that the relation between fraction of emerging Gibbs states and Brody parameter is universal.

The present results are also expected to have significant implications for the lively debated issue of thermalization in finite quantum systems [11, 13–15]. In this paper, we consistently avoided this notion and, instead, focused on thermal equilibrium states as we deduce the canonical density matrix from stationary energy eigenstates bypassing any explicit time dependence of the dynamics. Thermalization of an initial non-equilibrium state is, by contrast, a fundamental probe of the time evolution of quantum many-body systems. It will be of considerable interest to explore the imprint of the transition from quantum integrability to quantum chaos on the dynamics of out-of-equilibrium states. Most importantly, will quantum chaos play an analogous role for the process of mixing as classical chaos does for classical non-equilibrium dynamics and the relaxation to equilibrium? The origin and mechanism of such “quantum mixing” remains a widely open question.

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