Generalized Gibbs ensemble prediction of prethermalization plateaus and their relation to nonthermal steady states in integrable systems

Marcus Kollar, F. Alexander Wolf, and Martin Eckstein

1Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany
2Institute of Theoretical Physics, ETH Zurich, Wolfgang-Pauli-Str. 27, 8093 Zurich, Switzerland

(April 23, 2013)

A quantum many-body system which is prepared in the ground state of an integrable Hamiltonian does not directly thermalize after a sudden small parameter quench away from integrability. Rather, it will be trapped in a prethermalized state and can thermalize only at a later stage. We discuss several examples for which this prethermalized state shares some properties with the nonthermal steady state that emerges in the corresponding integrable system. These examples support the notion that nonthermal steady states in integrable systems may be viewed as prethermalized states that never decay further. Furthermore we show that prethermalization plateaus are under certain conditions correctly predicted by generalized Gibbs ensembles, which are the appropriate extension of standard statistical mechanics in the presence of many constants of motion. This establishes that the relaxation behaviors of integrable and nearly integrable systems are continuously connected and described by the same statistical theory.

I. INTRODUCTION

Quantum statistical mechanics can successfully predict the equilibrium properties of a system with many degrees of freedom, based only on a few macroscopic parameters such as energy, volume, and particle number. These predictions are obtained as averages over an ensemble of identical systems in which, according to the fundamental postulate of statistical mechanics, each accessible microscopic state is equally probable. The ensemble is described by a statistical operator $\hat{\rho}$ (with $\text{Tr}[\hat{\rho}] = 1$) which maximizes the entropy $S = -\text{Tr}[\hat{\rho} \ln \hat{\rho}]$. In the microcanonical ensemble $\hat{\rho}$ projects onto states with the correct macroscopic energy, but energy or other constants of motion can also be fixed only on average, as in the canonical or grand-canonical Gibbs ensemble. For macroscopic systems, the difference between the predictions of these standard ensembles is usually negligible, and they all describe the thermal state of the system in equilibrium. The statistical prediction for the equilibrium expectation value of an observable $\hat{A}$ is then $\text{Tr}[\hat{\rho} \hat{A}]$.

An ensemble describes a superposition of quantum states with classical probabilities and hence is a mixed state for which $\text{Tr}[\hat{\rho}^2] < 1$. Microscopically, however, a quantum system with Hamiltonian $H(t)$ evolves according to the Schrödinger equation, $\frac{i\hbar}{\Delta t} |\psi(t)\rangle = H(t)|\psi(t)\rangle$. It is described by the density matrix $\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)|$, i.e., a pure state with $\text{Tr}[\hat{\rho}(t)^2] = 1$. This leads to the question how a disrupted quantum system can ever thermalize, i.e., relax to a new equilibrium state which is described by a thermal ensemble with $\text{Tr}[\hat{\rho}^2] < 1$, although this quantity is constant during the unitary time evolution. There are two principal physical resolutions to this apparent mathematical paradox: (i) If the system is in contact with a (typically much larger) environment and only observables of the system are of interest, then the environment degrees of freedom can be traced out from $\hat{\rho}(t)$, leading to an effective statistical operator of the system that describes a mixed state. (ii) If the system is isolated (as we assume here), then due to many-body interactions in the Hamiltonian the time evolution of $|\psi(t)\rangle$ can be sufficiently ‘ergodic’ that for certain observables $\hat{A}$ the long-time limit of $\langle \hat{A}\rangle_t = \langle \psi(t)|\hat{A}|\psi(t)\rangle$ indeed tends to the statistical prediction $\text{Tr}[\hat{\rho} \hat{A}]$. Several possibly related concepts were developed to understand this behavior: Inspired by von Neumann’s quantum ergodic theorem, the theory of typicality puts bounds on the contributions to $\langle \hat{A}\rangle_t$ that are far from the thermal value. The eigenstate thermalization hypothesis puts bounds on the contributions to $\langle \hat{A}\rangle_t$ that are far from the thermal value. The eigenstate thermalization hypothesis can also be related to the many-body localization transition. However, thermalization has been related to the many-body localization transition.

Recent progress in the manipulation of cold atomic gases has made it possible to prepare quantum many-body systems in excellent isolation from the environment and to study their relaxation for a time-dependent Hamiltonian, thus providing a laboratory realization of the situation (ii) above. In particular, oscillations between Bose-condensed and Mott-insulating states after a deep sudden increase of the optical lattice depth were observed. In one-dimensional bosonic gases the dynamics leading to thermalization were measured for two coherently split gases and for a patterned initial state. On the other hand, a nonthermal steady state was reached for a one-dimensional trap in which the system is close to an integrable point. These developments have led to many theoretical studies regarding the relaxation of isolated quantum many-body systems (for recent reviews, see Refs. 29–31). In the simplest setup, a quantum many-body system is studied after a sudden parameter change...
(“quench”). In this situation the time evolution for \( t \geq 0 \) is governed by a time-independent Hamiltonian \( \hat{H} \), but the initial state at \( t = 0 \) is not an eigenstate of \( \hat{H} \). Rather the system is typically prepared in the ground state or a thermal state of some other initial Hamiltonian \( \hat{H}_0 \). Regarding the behavior of isolated interacting quantum systems after a global quench, three main cases can be distinguished: (a) Integrable systems which relax to a nonthermal steady state,\(^{28-44}\) which often can be described by generalized Gibbs ensembles (GGE) that take their large number of constants of motion into account.\(^{1,2,34}\) (b) nearly integrable systems that do not thermalize directly, but instead are trapped in a prethermalized state on intermediate timescales, which can be predicted from perturbation theory;\(^{45-48}\) and (c) nonintegrable systems which thermalize directly.\(^{13,27,36,47,49}\) We review these three cases in Sec. II.

Fig. 1 shows two examples for the cases (a) and (b) for which the transient behavior is qualitatively rather similar. In particular, both the integrable and the nearly integrable system enter a long-lived nonthermal state. This leads us to the question whether and how the two cases are related and which properties they share. Our main claim in this article is that (a) nonthermal steady states in integrable systems and (b) prethermalized states in nearly integrable systems are in precise correspondence, in the sense that both these nonthermal states are due to the existence of exact (in case (a)) or approximate (in case (b)) constants of motion (see Table I). We support this claim by two types of evidence. On the one hand (Sec. IIIA) we discuss several examples for which the predicted prethermalization plateau of an observable, when evaluated for an integrable system, yields precisely its nonthermal stationary value. In other words, nonthermal steady states in integrable systems can be understood as prethermalized states that never decay. On the other hand (Sec. IIIB) we obtain perturbed constants of motion that are approximately conserved in a nearly integrable system, use them to construct the corresponding GGE, and show that it describes the prethermalization plateau for a certain class of observables.\(^{50}\) It follows that integrable and nearly integrable systems are connected in the sense that their relaxation dynamics involve long-lived nonthermal states that are described by the same statistical theory.

II. INTEGRABILITY VS. THERMALIZATION

A. Integrable systems: Nonthermal steady states

If \( \hat{H} \) is integrable it has a large number of constants of motion, and the system then usually relaxes to a nonthermal steady state.\(^{28-44}\) This behavior is due to the fact that expectation values of all the constants of motion do not change with time. Therefore not all microstates in the relevant energy shell are in fact accessible, so that the above-mentioned fundamental postulate of statistical mechanics cannot be expected to give a reliable description of the steady state. In contrast to the classical case it is not obvious whether a given Hamiltonian is integrable, because any quantum Hamiltonian \( \hat{H} \) always has as many constants of motion as the dimension of the Hilbert space, e.g., its powers, or the projectors onto its eigenstates.\(^{13,37,51,52}\) Many solvable Hamiltonians \( \hat{H} \), however, are integrable in a stronger sense, namely they can be mapped, \( \hat{H} \rightarrow \hat{H}_{\text{eff}} \), onto a effective Hamiltonian of the form

\[
\hat{H}_{\text{eff}} = \sum_{\alpha=1}^{L} \epsilon_\alpha \hat{T}_\alpha ,
\]

with \( [\hat{T}_\alpha, \hat{T}_\beta] = 0 \) for all \( \alpha \) and \( \beta \) and thus \( [\hat{H}, \hat{T}_\alpha] = 0 \), where \( \hat{L} \) is proportional to the system size rather than
TABLE I. Nonthermal (quasi-)stationary states after a quench to an integrable or nearly integrable Hamiltonian $\hat{H}$. 

| Case                  | Hamiltonian $\hat{H}$ after quench | (quasi-)stationary state                                      |
|-----------------------|------------------------------------|-------------------------------------------------------------|
| (a) integrable case   | $\hat{H}$ integrable with exact constants of motion | nonthermal steady state in the long-time limit, $t \to \infty$ |
| (b) nearly integrable case | $\hat{H} = \hat{H}_0 + g\hat{H}_1$, $|g| < 1$, $\hat{H}_0$ integrable, $\hat{H}$ not integrable with approx. constants of motion | prethermalized state for intermediate times $t$ with $|g|^{-1} \ll \text{const} \cdot t \ll g^{-2}$ |

The purpose of these additional constraints is to take into account (on average) that many microstates are inaccessible during the time evolution because they are incompatible with the values of the conserved quantities in the initial state. GGEs correctly predict many (but not all) properties of nonthermal steady states in various integrable models. A microcanonical analogue of Eq. (2), the so-called generalized microcanonical ensemble, was also studied.

**B. Nearly integrable systems: Prethermalization**

Now consider the case that the Hamiltonian $\hat{H}$ after the quench is not exactly integrable but close to an integrable point with Hamiltonian $\hat{H}_0$, i.e.,

$$\hat{H} = \hat{H}_0 + g\hat{H}_1,$$

(3a)

$$\hat{H}_0 = \sum_{\alpha} \epsilon_\alpha \hat{\mathcal{I}}_\alpha,$$

(3b)

with $|g| < 1$, i.e., now the full Hamiltonian $\hat{H}$ is almost but not exactly of the form (1). In this case the relaxation dynamics is nevertheless strongly influenced by the near-integrability, i.e., due to the presence of approximate constants of motion, as discussed in more detail below. In such cases the system prethermalizes, i.e., $\langle \hat{A} \rangle$ relaxes first to a nonthermal quasistationary value $A_{\text{stat}}$ that is increasingly long-lived as $\hat{H}$ approaches the integrable point at $g = 0$. One of the characteristic features of prethermalization, known from field theory, is that integrated quantities such as kinetic and potential energy attain their thermal values much earlier than individual occupation numbers. This phenomenon was recently studied in detail for Fermi liquids by Mocek and Kehrein, namely for interaction quenches from $U = 0$ to small values of $U > 0$ in the fermionic Hubbard model with Hamiltonian

$$\hat{H} = \sum_{ij\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

(4)

which for $U = 0$ reduces to an integrable Hamiltonian (3b) in which the momentum occupation numbers $\hat{n}_{k\sigma} = \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma}$ play the role of the conserved quantities $\hat{\mathcal{I}}_\sigma$.

It was stressed in Ref. 46 that in analogy to classical mechanics naive perturbation theory leads to secular terms that grow polynomially in time; instead instead one should use unitary perturbation theory, i.e., absorb the perturbation by a unitary transformation, perform the time evolution, and transform back. In Appendix A we derive a simple form of unitary perturbation theory (already used in Ref. 46) for a nondegenerate Hamiltonian $\hat{H}_0$. If the time evolution is governed by the a nearly integrable Hamiltonian $\hat{H}$ [Eq. (3)], we obtain the expectation value of an observable $\hat{A}$ as (see Appendix B1)

$$\langle \hat{A} \rangle_t = \langle \hat{A} \rangle_0 + 4g^2 \int_{-\infty}^{\infty} d\omega \frac{\sin^2(\omega t/2)}{\omega^2} J(\omega) + O(g^3),$$

(5)

where the function $J(\omega)$ depends on the observable $\hat{A}$ and the initial state $|\psi(0)\rangle$. In the case that (i) $\hat{A}$ commutes
with all constants of motion \( \hat{L}_\alpha \) and (ii) the initial state \( |\psi(0)\rangle \) is an eigenstate of \( \hat{H}_0 \), it can be written as

\[
J(\omega) = \langle \hat{H}_1 (\hat{A} - \langle \hat{A} \rangle_0) \delta(\hat{H}_0 - \langle \hat{H}_0 \rangle - \omega) \hat{H}_1 \rangle_0. \tag{6}
\]

These two assumptions (i) and (ii) are merely made to obtain the compact result (6); it is straightforward to extend the analysis to any observable and any initial state. We note that an evaluation (see Appendix B.2) of \( \langle \hat{n}_{k\sigma} \rangle_t \) according to Eqs. (5-6) for quenches from 0 to small \( U \) in the fermionic Hubbard model [Eq. (4)] recovers the result obtained with flow equations for continuous unitary transformations.\(^{46}\) The prethermalization plateau, denoted by \( A_{\text{stat}} \), can be obtained as the long-time average of Eq. (5), \( \lim_{t \to \infty} \int_0^t dt' / t \langle \hat{A} \rangle_{t'} \), assuming that \( |g| \) is so small that the scales \( 1/|g| \) and \( 1/g^2 \) are well separated and the limit \( t \to \infty \) is taken in the sense that \( 1/|g| \ll \text{const} \cdot t \ll 1/g^2.\)\(^{46}\)

\[
A_{\text{stat}} = \langle \hat{A} \rangle_0 + 2g^2 \int_{-\infty}^{\infty} d\omega \omega^2 J(\omega) + O(g^3). \tag{7}
\]

If \( \hat{A} \) commutes with all \( \hat{L}_\alpha \) and \( |\psi(0)\rangle \) is an eigenstate of \( \hat{H}_0 \), this expression simplifies to

\[
A_{\text{stat}} = 2\langle \hat{A} \rangle_0 - \langle \hat{A} \rangle_0 + O(g^3), \tag{8}
\]

where \( \langle \hat{A} \rangle_0 = \langle \tilde{\psi}(0)|\hat{A}|\tilde{\psi}(0)\rangle \) denotes the expectation value in the perturbative eigenstate \( |\tilde{\psi}(0)\rangle \) of \( \hat{H} \) corresponding to the initial state \( |\psi(0)\rangle \).\(^{46}\)

In general \( A_{\text{stat}} \) differs from the thermal expectation value of \( \hat{A} \) obtained with a microcanonical or canonical ensemble with the same average energy \( E \) as the quenched system, i.e., \( E = \langle \tilde{\psi}(0)|\hat{H}|\tilde{\psi}(0)\rangle = \langle \tilde{\psi}(t)|\hat{H}|\tilde{\psi}(t)\rangle \). Hence if subsequent thermalization occurs it is expected to be due to processes of order \( g^3 \) and higher and to happen at later times, \( t \gg 1/g^2 \).\(^{46,48,61}\) The prethermalization plateau (8) and also the predicted transient behavior (5)\(^{46}\) were confirmed for \( \hat{n}_{k\sigma} \) after interaction quenches in the Hubbard model in DMFT;\(^{47}\) later-stage relaxation towards the thermal values was also observed (see also Fig. 1b).

### C. Nonintegrable systems: Thermalization

For nonintegrable systems thermalization is expected for sufficiently long times because only few relevant constants of motion exist, and was observed in several systems.\(^{13,27,36,47,49}\) Due to limitations in simulation time and/or system size it is sometimes difficult to determine whether the required distance from an integrable point for which thermalization occurs is finite (as suggested, e.g., by the results of Refs. 36, 37, and 62) or infinitesimal in the thermodynamic limit (as suggested by a general analysis in Ref. 61) This issue, as well as the mechanism for thermalization, is still being developed and debated.\(^{3-23,63}\) Interestingly, signatures of thermalization were also found for certain variables in integrable systems.\(^{64}\)

### III. INTEGRABLE VS. NEARLY INTEGRABLE SYSTEMS

Our main claim in this article is the close correspondence between (a) nonthermal stationary values in integrable systems, i.e., \( \langle \hat{A} \rangle_\infty = \lim_{t \to \infty} \langle \hat{A} \rangle_t \), and (b) prethermalization plateaus \( A_{\text{stat}} \) in nearly integrable systems. In Sec. III A we discuss several examples for which the predicted prethermalization plateau of an observable (7), when evaluated for an integrable system of type (1), yields precisely its nonthermal stationary value. We then obtain in Sec. III B that prethermalized states are described by an appropriate GGE built from approximate constants of motion, analogous to nonthermal steady states in integrable systems that are described by a GGE built from exact constants of motion.

#### A. Nonthermal steady states in integrable systems are prethermalized states that never decay

We now compare the two values \( A_{\text{stat}} \) [Eq. (7)] and \( \langle \hat{A} \rangle_\infty \) analytically or to high numerical accuracy for interaction quenches to weak and strong coupling in two Hubbard-type models, namely in the \( 1/r \) Hubbard chain\(^{41}\) and the Falicov-Kimball model in DMFT (i.e., in the limit of infinite spatial dimensions),\(^{40,42}\) which are integrable in the sense of Eq. (1). For both models the Hamiltonian is of the form (4) (however, for the Falicov-Kimball model the hopping amplitude is zero for one of the spin species). As observable we consider the double occupation \( \bar{d} = \langle \sum_i \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} \rangle / L \) (\( L \): number of lattice sites). We obtain \( d_{\text{stat}} \) from Eq. (7) for these two integrable systems, and show that it agrees with the nonthermal stationary value \( \langle \bar{d} \rangle_\infty \).

1. Weak coupling

We first consider an interaction quench from 0 to small values of \( U \). Then the prethermalization plateau of \( \bar{n}_{k\sigma} \) is given by Eq. (8), and \( d_{\text{stat}} \) can be obtained using energy conservation after the quench. For the integrable \( 1/r \) Hubbard chain (with bandwidth \( W \) and particle density \( n \leq 1 \)) we use known properties of the perturbed ground state \( |\tilde{\psi}(0)\rangle \) and obtain (see Appendix C)

\[
d_{\text{stat}} = \frac{n^2}{4} - \frac{n^2(3-2n)U}{6W} + O(U^2). \tag{9}
\]

When comparing this predicted prethermalization plateau with the exact long-time limit \( \langle \bar{d} \rangle_\infty \) (Ref. 41)
we see that both values agree to order $U$ for all densities $n \leq 1$. For this integrable system Eq. (8) thus predicts the nonthermal stationary value instead of a prethermalization plateau.

2. Strong coupling

For interaction quenches from 0 to large values of $U$ the final Hamiltonian is also close to an integrable point, namely the atomic limit with conserved occupation numbers $\hat{c}_i^\dagger \hat{c}_i$ on each lattice site. However, we consider an initial Hamiltonian other than the atomic limit, so that Eqs. (6) and (8) do not apply. Instead, $d_{\text{stat}}$ is given by unitary strong-coupling perturbation theory\textsuperscript{47,65} as

$$d_{\text{stat}} = \langle \hat{d} \rangle_0 + \sum_{ij\sigma} \frac{t_{ij\sigma}}{UL} \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} (\hat{n}_{i\bar{\sigma}} - \hat{n}_{j\bar{\sigma}})^2 \rangle_0 + O(U^{-2}),$$

valid for an arbitrary initial state $|\psi(0)\rangle$. We note that for a nonintegrable system $d_{\text{stat}}$ was observed as the center of collapse-and-revival oscillations that occur after interaction quenches to large $U$ in the Hubbard model in DMFT.\textsuperscript{47}

For quenches from $U = 0$ to large $U$ in the integrable 1/r Hubbard model Eq. (10) predicts:\textsuperscript{47}

$$d_{\text{stat}} = \frac{n^2}{4} - \frac{2(3 - 2n)W}{3U} + O(U^{-2}).$$

Comparing this prediction with the exact long-time limit $\langle \hat{d} \rangle_\infty$ (Ref. 41) we find again that they are in agreement to order $U^{-1}$ for all densities $n \leq 1$.

Finally, for the Falicov-Kimball model in DMFT with a semielliptic density of states, the value $d_{\text{stat}}$ predicted by Eq. (10) is

$$d_{\text{stat}} = \frac{n^2}{4} - \frac{(2 - n)n}{2U} \langle \hat{H}_0 \rangle_0 + O(U^{-2}).$$

Fig. 2 shows the exact double occupation $\langle \hat{d} \rangle_t$ for the Falicov-Kimball model in DMFT for quenches from 0 to large $U$. In the long-time limit $\langle \hat{d} \rangle_t$ tends precisely to the predicted value (12) in the long-time limit large $U$.

3. Summary

For these three examples of integrable Hubbard-type systems we showed that prethermalized states, described by unitary perturbation theory for nearly integrable systems, also describes the nonthermal steady state in integrable systems. This suggests the viewpoint that nonthermal steady states in integrable systems are simply prethermalized states that never decay. In other words, the system appears to be trapped in essentially the same state both at and very close to an integrable point. This suggests that the prethermalized state approaches the nonthermal steady state as one quenches closer and closer to the integrable point. We cannot show this continuity in general, but provide a continuous statistical description of integrable and nonintegrable systems in the next subsection.

B. Construction of approximate constants of motion for nearly integrable systems and the corresponding generalized Gibbs ensemble

We now turn to the question whether for a small quench from an integrable point $\hat{H}_0$ to $\hat{H} = \hat{H}_0 + g\hat{H}_1$ (with $|g| \ll 1$) the prethermalization plateau (8) is described by an appropriate Gibbs ensemble involving approximate constants of motion. We use the eigenbasis $|\mathbf{n}\rangle$ of the constants of motion, i.e., $\mathbf{n} = (n_1, n_2, \ldots, n_L)$,
\( \hat{I}_\alpha |n\rangle = n_\alpha |n\rangle \), and assume that the energies \( \epsilon_\alpha \) are incommensurate, so that the eigenenergies \( E_n = \sum_\alpha \epsilon_\alpha n_\alpha \) of \( \hat{H}_0 \) are nondegenerate. This is not a strong restriction as the boundaries of the system can always be imagined to be so irregular as to lift all degeneracies.

As described in Appendix A a unitary transformation \( e^S \) can be constructed which yields

\[
\hat{H} = \sum_\alpha \epsilon_\alpha \hat{I}_\alpha + \sum_n \langle n | (g E_n^{(1)} + g^2 E_n^{(2)}) | n \rangle + O(g^3), \tag{13a}
\]

\[
\hat{I}_\alpha = e^{-S} \hat{I}_\alpha e^S
\]

\[
= \hat{I}_\alpha - [\hat{S}, \hat{I}_\alpha] + [\hat{S}, [\hat{S}, \hat{I}_\alpha]] + O(g^3), \tag{13b}
\]

where \( \hat{H}|\tilde{n}\rangle = \tilde{E}_n |\tilde{n}\rangle \), \( |\tilde{n}\rangle = e^{-\hat{S}} |n\rangle \), and \( E_n^{(1,2)} \) are the standard energy corrections in first and second order perturbation theory, recovering the perturbed Rayleigh-Schrödinger energy eigenvalues,

\[
\tilde{E}_n = E_n + g E_n^{(1)} + g^2 E_n^{(2)} + O(g^3). \tag{14}
\]

The structure of the transformed Hamiltonian is plausible: the first term on the left-hand side in Eq. (13a) retains the additive ‘noninteracting’ structure of the integrable Hamiltonian \( \hat{H}_0 \) with the same ‘one-particle’ energies \( \epsilon_\alpha \), whereas the perturbative energy corrections are not additive in this way but rather depend explicitly on the configuration of the state \( e^{-S} |n\rangle \). Other perturbed Hamiltonians with a different structure were proposed in the literature, e.g., with modified energies \( \tilde{\epsilon}_\alpha \), or perturbed energy eigenvalues \( \tilde{E}_n \) that remain additive in the quantum numbers \( n_\alpha \).

Since \( [\hat{I}_\alpha, \hat{I}_\beta] = [\hat{I}_\alpha, \hat{I}_\beta] = 0 \) we have \( [\hat{H}, \hat{I}_\alpha] = O(g^3) \), so that the \( \hat{I}_\alpha \) are the desired approximate constants of motion that indeed commute with \( \hat{H} \) to order \( g^3 \). Note that in principle our canonical transformation can be continued to arbitrary high order in \( g \), but an accurate description can nevertheless only be expected in a perturbative regime of sufficiently small \( g \). Next we construct the corresponding GGE with these perturbed constants of motion,

\[
\hat{\rho}_G = \frac{1}{Z_G} \exp \left( - \sum_\alpha \lambda_\alpha \hat{I}_\alpha \right), \tag{15}
\]

where the \( \lambda_\alpha \) are fixed by the initial state according to

\[
\langle \hat{I}_\alpha \rangle_G = \text{Tr}[\hat{\rho}_G \hat{I}_\alpha] \equiv \langle \hat{I}_\alpha \rangle_0. \tag{16}
\]

Here we choose only the conserved quantities \( \hat{I}_\alpha \) that appear linearly and additively in the Hamiltonian (13a) to construct the GGE. Note that the Hamiltonian (13a) is not precisely of the form (1) but rather contains additional diagonal terms that involve the projectors \( |\tilde{n}\rangle \langle \tilde{n}| \).

These projectors are in general nonlinear in the \( \hat{I}_\alpha \) and are therefore not used in the GGE: the use of products of conserved quantities in the GGE is discussed in Refs. 13, 38, and 41, but not pursued here.

We now come to the central point of this article: we compare the prethermalization plateau of \( \hat{H}_0 \) (which are no longer conserved during the time evolution with \( \hat{H} = \hat{H}_0 + g \hat{H}_1 \)) is predicted correctly in order \( g^2 \) by the appropriate statistical theory [Eq. (15)]. Hence on timescales \( 1/|g| \ll \text{const} \cdot t \ll 1/g^2 \) the pure state \( |\psi(t)\rangle \) gives the same expectation values as a mixed state described by \( \hat{\rho}_G \). For a more complicated observable,

\[
\hat{A} = \prod_{i=1}^n \hat{I}_{\alpha_i},
\]

we also find

\[
\hat{A}_{\text{stat}} = \langle \hat{A} \rangle_G + O(g^3),
\]

provided the condition

\[
\langle \prod_{i=1}^n \hat{I}_{\alpha_i} \rangle_0 = \prod_{i=1}^n \langle \hat{I}_{\alpha_i} \rangle_0 + O(g^3)
\]

is fulfilled. This is due to the fact that the GGE \( \hat{\rho}_G \) is diagonal in the \( \hat{I}_\alpha \) and therefore cannot describe arbitrary correlations that are built up between two or more \( \hat{I}_{\alpha_i} \), which is a well-known limitation. \(^{38,39,41}\) At the integrable point \( g = 0 \) and \( |\psi(0)\rangle = |\tilde{\psi}(0)\rangle \) the factorization condition (20) reduces to the condition derived in Ref. 41 for the validity of a GGE (2) for an integrable Hamiltonian (1).

The above assumption about the structure of \( \hat{H}_1 \) ensures that it does not contain operators that are absent in \( \hat{\rho}_G \). Information about such operators would be missing from the GGE ensemble (15), making their correct
description unlikely. However, this is not a strong restriction, as several coupled spaces can also be considered in a GGE (see, e.g., Ref. 44).

We conclude that the phenomenon of prethermalization not only means that a long-lived nonthermal state is attained prior to possible thermalization at a later stage, but also that the properties of the prethermalized state are predicted correctly by an ensemble that is constructed according to the principles of statistical mechanics.

IV. CONCLUSION

We argued that integrable and nearly integrable systems are continuously connected in the following sense: (a) Integrable systems relax to nonthermal, but GGE-described stationary states; (b) Near-integrable systems are trapped in quasistationary states due to the perturbed constants of motion of the nearby integrable system, and can also be described by an appropriate perturbed GGE. Hence if one studies the relaxation of a nonintegrable system closer and closer to an integrable point, the prethermalization plateau will survive longer and longer and will approach the nonthermal long-time limit at the integrable point, with the appropriate GGE describing this steady state throughout.

Previously GGEs were only used to describe integrable systems. Here we showed that GGEs can make valid predictions also away from integrable points, at least perturbatively. In our opinion this illustrates the power of statistical mechanics, which makes correct predictions provided that the observables are not too complicated and only the accessible phase space is included in the statistical operator.

Acknowledgements. Insightful discussions with Stefan Kehrein, Michael Moeckel, Anatoli Polkovnikov, Marcos Rigol, Mark Srednicki, Michael Stark, Leticia Tarruell, Dieter Vollhardt, David Weiss, and Philipp Werner are gratefully acknowledged. This work was supported in part by DFG (SFB 484, TRR 80).
The transformed Hamiltonian shall still have all \( \hat{C} \) constants of motion, i.e., we demand

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APPENDIX

Appendix A: Unitary perturbation theory

We use a canonical transformation \( e^{\hat{S}} \), similar to Ref. 46, which reproduces second-order Rayleigh-Schrödinger perturbation theory at the operator level and thus enables us to construct the approximate constants of motion of \( \hat{H} = \hat{H}_0 + g\hat{H}_1 \). We expand the antihermitian operator \( \hat{S} \) in powers of \( g \),

\[
\hat{S} = g\hat{S}_1 + \frac{1}{2} g^2 \hat{S}_2 + O(g^3), \quad (A1)
\]

and apply the canonical transformation to \( \hat{H} \),

\[
e^{\hat{S}} \hat{H} e^{-\hat{S}} = \hat{H}_0 + g(\hat{H}_1 + [\hat{S}_1, \hat{H}_0]) + g^2 \left( \frac{1}{2} [\hat{S}_2, \hat{H}_0] + \frac{1}{2} [\hat{S}_1, [\hat{S}_1, \hat{H}_0]] \right) + O(g^3). \quad (A2)
\]

The transformed Hamiltonian shall still have all \( \hat{T}_\alpha \) as constants of motion, i.e., we demand \( [e^{\hat{S}} \hat{H} e^{-\hat{S}}, \hat{T}_\alpha] = 0 \) for all \( \alpha \), order by order. We use the basis \( \hat{T}_\alpha | n \rangle = n_\alpha | n \rangle \) and assume that the energies \( \epsilon_\alpha \) are incommensurate, so that the eigenenergies \( E_n = \sum_\alpha \epsilon_\alpha n_\alpha \) of \( \hat{H}_0 \) are nondegenerate. To second order in \( g \) we obtain for the transformed Hamiltonian and the unitary transformation

\[
\begin{align*}
\hat{H}_{\text{diag}} &= e^{\hat{S}} \hat{H} e^{-\hat{S}} = \hat{H}_0 + g\hat{H}_{1,\text{diag}} + g^2 \hat{H}_{2,\text{diag}} + O(g^3), \\
(n|\hat{S}_1|m) &= \begin{cases} 
\frac{\langle n|\hat{H}_1|m \rangle}{E_n - E_m} & \text{if } n \neq m \\
0 & \text{if } n = m 
\end{cases}, \\
\langle n|\hat{S}_2|m \rangle &= \begin{cases} 
\frac{\langle n|\hat{S}_1, H_1 + \hat{H}_{1,\text{diag}}|m \rangle}{E_n - E_m} & \text{if } n \neq m \\
0 & \text{if } n = m 
\end{cases}, \\
\hat{H}_{1,\text{diag}} &= \sum_n |n\rangle E_n^{(1)} \langle n |, \\
E_n^{(1)} &= \langle n|\hat{H}_1|m \rangle, \\
E_n^{(2)} &= \sum_{m \neq n} \frac{|\langle m|\hat{H}_1|m \rangle|^2}{E_n - E_m},
\end{align*}
\]

from which the eigenvalues \( \bar{E}_n \) [Eq. (14)] of the eigenstates \( |n\rangle = e^{-\hat{S}} |n\rangle \) can be read off.
Appendix B: Transients in nearly integrable systems

1. Derivation of Eqs. (5), (6), (8)

Here we obtain the transient behavior in second order unitary perturbation theory, in close analogy to the derivation in Ref. 46. We assume that the initial state is an eigenstate of ̂H₀,

\[ |\psi(0)⟩ = |p⟩, \]  

(B1)

\[ ̂J_α|p⟩ = p_α|p⟩, \]  

and that the observable ̂A commutes with all constants of motion ̂J_α. For now we set ⟨A⟩₀ = 0 and reinstate a possibly nonzero initial value at the end. Inserting the unitary transformation for the Hamiltonian we obtain

\[ ⟨A⟩_t = ⟨p|e^{i ̂H t} ̂A e^{-i ̂H t}|p⟩ \]  

(B2)

with the abbreviation ̂S(t) = e^{i ̂Hdiag t} ̂S e^{-i ̂Hdiag t}. Expanding the inner transformation as

\[ e^{i ̂S(t)} ̂A e^{-i ̂S(t)} = A + [S(t), A] + \frac{1}{2} [S(t), [S(t), A]] + O(g^3) \]  

(B3)

and then similarly expanding the outer back transformation, we have

\[ ⟨A⟩_t = \langle p| ̂A + [ ̂S(t) − ̂S, ̂A] − \frac{1}{2} [ ̂S, [ ̂S(t) − ̂S, ̂A]] \]  

\[ + \frac{1}{2} [ ̂S(t), [ ̂S(t), ̂A]]|p⟩ + O(g^3) \]  

(B4)

Here and below we frequently use that ̂A annihilates |p⟩, ̂A commutes with ̂Hdiag, and |p⟩ is an eigenstate of ̂Hdiag. In the second term of the last equation we can rewrite

\[ \langle p| ̂S ̂A ̂S(t)|p⟩ \]  

\[ = − \sum_{n(\neq p)} |⟨p| ̂S|n⟩|^2 |⟨n| ̂A|n⟩| e^{-i(E_p − E_n)t} \]  

\[ = − \sum_{n(\neq p)} |⟨p| ̂H|n⟩|^2 |⟨n| ̂A|n⟩| e^{-i(E_p − E_n)t} + O(g^3) \]  

\[ = −2g^2 \int_{−∞}^{∞} dω J(ω) e^{iωt} + O(g^3). \]  

(B5)

Here we have defined

\[ J(ω) = \sum_{n(\neq p)} |⟨p| ̂H|n⟩|^2 |⟨n| ̂A|n⟩|δ(ω − (E_n − E_p)) \]  

\[ = ⟨p| ̂H ̂A δ(ω − ( ̂H₀ − ⟨ ̂H₀⟩)) ̂H₀|p⟩, \]  

as in Eq. (6). By setting t = 0 in Eq. (B5) we obtain a similar expression for the first term in Eq. (B4), which leads to Eq. (8). Eq. (B5) then also yields

\[ ⟨ ̂A⟩_t = g^2 \int_{−∞}^{∞} dω J(ω) \frac{4 sin^2(ωt/2)}{ω^2} + O(g^3), \]  

(B7)

as in Eq. (5).

2. Evaluation for a small two-body interaction quench in a Fermi gas

Here we evaluate the function J(ω) for a two-body interaction quench, i.e.,

\[ ̂H₀ = \sum_α ε_α c_α^† c_α, \quad ̂H₁ = \sum_{αβγδ} V_{αβγδ} c_α^† c_β^† c_γ c_δ, \]  

(B8)

for fermionic operators, \{c_α, c_α^†\} = δ_αβ and \{c_α, c_β\} = 0; hence V_{αβγδ} = −V_{βαγδ} = −V_{αβδγ} = V_{βαδγ} and V_{αβγδ} = = (V_{γδβα})*. The occupation numbers \hat{n}_α = c_α^† c_α (with eigenvalues 0, 1) play the role of constants of motion \hat{Ł}_α of the unperturbed system (a Fermi gas) before the quench. As observable we choose the change in the occupation number of a state µ,

\[ A = ̂Ł_μ − ( ̂Ł_μ)|p⟩ = \hat{n}_µ − p_µ, \]  

(B9)

where |ψ(0)⟩ = |p⟩ is the initial state with \hat{Ł}_α|p⟩ = p_α|p⟩.

\[ J(ω) = \sum_{αβγδ} V_{αβγδ} (p)|c_α^† c_β^† c_γ c_δ|e^{i(ω−δ_μ)−E_p} \]  

\[ − p_µ \sum_{αβγδ} 4V_{μβγδ} c_α^† c_β^† c_γ c_δ|p⟩, \]  

(B10)

where \hat{Ł}_0 − E_p inside the delta function evaluates to ε_α + ε_β − ε_γ − ε_δ. In the initial state the single-particle level µ may be occupied (p_µ = 1) or unoccupied (p_µ = 0), and inside the sum the operator (\hat{n}_µ − p_µ) must yield a nonzero contribution. We consider first p_µ = 1, in which case this requirement leads to a factor

\[ (δ_μ(1 − δ_β) + δ_β(1 − δ_µ))(1 − δ_α)(1 − δ_δ)\]  

\[ \times (1 − δ_γ)(1 − δ_δ)(1 − δ_α)(1 − δ_β)\]  

× \[ (1 − δ_α)(1 − δ_δ)(1 − δ_γ)(1 − δ_δ), \]  

Using the symmetries of V_{αβγδ} we obtain the following contribution to J(ω),

\[ − p_µ \sum_{αβγδ} 4V_{μβγδ} c_α^† c_β^† c_γ c_δ|p⟩, \]  

(B11)

Next for p_µ = 0 we find the factor

\[ (δ_α(1 − δ_β) + δ_β(1 − δ_α))(1 − δ_δ)(1 − δ_δ)\]  

\[ \times (1 − δ_γ)(1 − δ_δ)(1 − δ_γ)(1 − δ_δ), \]  

\[ \times (1 − δ_α)(1 − δ_δ)(1 − δ_γ)(1 − δ_δ), \]  

(B12)
so that the contribution to $J(\omega)$ is

$$(1 - p_\mu) \sum_{\alpha\beta\gamma\delta' \in \{1, \ldots, \mu\}} 4V_{\mu\beta\gamma\delta} V_{\alpha'\beta'\gamma'\delta'} \times$$

$$\delta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\delta - \omega) \langle p | \hat{c}_\alpha^\dagger \hat{c}_\beta^\dagger \hat{c}_\gamma \hat{c}_\delta | p \rangle .$$  \hfill (B12)

Evaluating the expectation values in Eqs. (B11) and (B12) in the product state $| p \rangle$ by contractions we finally obtain

$$J(\omega) =$$

$$- p_\mu \left[ 16 \sum_\alpha (1 - p_\alpha) |W_{\alpha\mu}|^2 \delta(\epsilon_\alpha - \epsilon_\mu - \omega)$$

$$+ 8 \sum_{\alpha\beta\gamma} |V_{\alpha\beta\gamma\delta}|^2 (1 - p_\alpha)(1 - p_\beta)p_\gamma$$

$$\times \delta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\mu - \omega) \right]$$

$$+ (1 - p_\mu) \left[ 16 \sum_\alpha p_\alpha |W_{\alpha\mu}|^2 \delta(\epsilon_\beta - \epsilon_\mu - \omega)$$

$$+ 8 \sum_{\alpha\beta\gamma} |V_{\alpha\beta\gamma\delta}|^2 (1 - p_\alpha)(1 - p_\beta)p_\gamma$$

$$\times \delta(\epsilon_\alpha + \epsilon_\beta - \epsilon_\gamma - \epsilon_\mu - \omega) \right],$$ \hfill (B13)

with the abbreviation

$$W_{\alpha\mu} = \sum_\beta V_{\alpha\beta\mu} p_\beta .$$  \hfill (B14)

For completeness we now evaluate Eq. (B13) for the observable $\hat{n}_{k\sigma}$ in the Hubbard model (4) by setting $\alpha = (k_1, \sigma_1)$ etc.,

$$V_{\alpha\beta\delta} = \frac{U}{4L} \Delta(k_1 + k_2 + k_3 + k_4)$$

$$\times \sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \delta_{\sigma_1\sigma_2} \delta_{\sigma_2\sigma_3} \delta_{\sigma_3\sigma_4} - \delta_{\sigma_1\sigma} \delta_{\sigma_4\sigma} ,$$ \hfill (B15)

so that in particular $V_{\alpha\beta\delta} = 0$, $W_{\alpha\mu} = 0$. Here $\Delta(k) = \sum_G \delta_{k,G}$ is the von-Laue function involving reciprocal lattice vectors $G$. Eq. (B13) then takes the form

$$J_{k\sigma}(\omega) = - \frac{U^2}{L^2} \sum_{k_1k_2k_3k_4} \Delta(k_1 + k_2 + k_3 + k_4)$$

$$\times \delta(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_3} - \epsilon_{k_4} - \omega)$$

$$\times \left[ (1 - p_{k_1,\sigma})(1 - p_{k_2,\sigma})p_{k_3,\sigma}p_{k_\sigma}$$

$$- p_{k_1,\sigma}p_{k_2,\sigma}p_{k_3,\sigma}(1 - p_{k_\sigma}) \right],$$ \hfill (B16)

where $p_{k\sigma}$ are the momentum occupation numbers in the initial state. When inserted into Eq. (5) this leads to the same expression for the transient behavior that Moeckel and Kehrein\textsuperscript{46} obtained using continuous unitary transformations, but here we used only a single unitary transformation.

**Appendix C: Properties of the weak-coupling ground state of the $1/r$ Hubbard chain**

For the $1/r$ Hubbard chain the kinetic energy per lattice site $\epsilon_{\text{kin}}(U)$ can be obtained from the fact that the ground-state energy is given by the variational Gutzwiller energy up to $O(U^2)$,\textsuperscript{58} which yields ($W$: bandwidth, $L = \text{number of lattice sites}$)

$$\epsilon_{\text{kin}}(U) = \frac{1}{L} \sum_{k\sigma} \epsilon_k (\hat{n}_{k\sigma}) \hat{\gamma}$$

$$= \frac{n(2 - n)W}{4} - \frac{n^2 (2n - 3)U^2}{12W} + O(U^3) .$$ \hfill (C1)

For a quench from 0 to $U$ the prethermalization plateau of each momentum occupation number $\hat{n}_{k\sigma}$ is given by Eq. (8). Using the fact that the total energy is conserved after the quench, the prethermalization plateau of the double occupation $\hat{d}$ is then given by

$$d_{\text{stat}} = \langle d \rangle_0 - \frac{2}{U} [\epsilon_{\text{kin}}(U) - \epsilon_{\text{kin}}(0)] + O(U^2) ,$$ \hfill (C2)

which, together with Eq. (C1), yields Eq. (9).

**Appendix D: GGE prediction for prethermalization plateaus [Derivation of Eqs. (17), (20)]**

In the following derivation of Eqs. (17), (20) we repeatedly use Eq. (16) which fixes the Lagrange multipliers. Several transformations between the eigenbases of the $\hat{I}_\alpha$ and the $\hat{\gamma}_\alpha$ are performed. We have

$$\langle \hat{A} \rangle_G = \frac{\text{Tr}[\hat{A} e^{-\sum_{\alpha} \lambda_\alpha \hat{I}_\alpha}]}{\text{Tr}[e^{-\sum_{\alpha} \lambda_\alpha \hat{I}_\alpha}]}$$

$$= \frac{\text{Tr}[e^{\hat{S}} \hat{A} e^{-\hat{S}} e^{-\sum_{\alpha} \lambda_\alpha \hat{I}_\alpha}]}{\text{Tr}[e^{-\sum_{\alpha} \lambda_\alpha \hat{I}_\alpha}]} = \langle e^{\hat{S}} \hat{A} e^{-\hat{S}} \rangle_G$$

$$= \langle \hat{A} + [\hat{S}, \hat{A}] + \frac{1}{2} [\hat{S}, [\hat{S}, \hat{A}]] \rangle_G + O(g^3) ,$$ \hfill (D1)

where $\langle \cdot \rangle_G$ denotes the GGE expectation value (2) but with the $\lambda_\alpha$ still fixed by Eq. (16). We proceed to evaluate the three terms in $\langle \hat{A} \rangle_G$ for an observable of the form (18). The first term can be rewritten as

$$\langle \hat{A} \rangle_G = \prod_{i=1}^m \langle \hat{I}_{\alpha_i} \rangle_G = \prod_{i=1}^m \langle \hat{I}_{\alpha_i} \rangle_\hat{\gamma} \prod_{i=1}^m \langle \hat{\gamma}_{\alpha_i} \rangle_\hat{\gamma}$$

$$= \prod_{i=1}^m \langle \hat{\gamma}_{\alpha_i} \rangle_\hat{\gamma} = \prod_{i=1}^m \langle \hat{\gamma}_{\alpha_i} \rangle_0 + O(g^3) ,$$ \hfill (D2)
the second term vanishes, and the third term becomes

\[
\langle \frac{1}{2}[\hat{S}, [\hat{S}, \hat{A}]] \rangle_G = \sum_n g^2 \langle n | \frac{1}{2}[\hat{S}_1, [\hat{S}_0, \hat{A}]] | n \rangle \frac{1}{Z_G} e^{-\sum \lambda_n n \lambda_n} + O(g^3)
\]

\[
= g^2 F(\{\{\tilde{\mathcal{I}}_0\}_G\}) + O(g^3)
\]

\[
= g^2 F(\{\{\tilde{\mathcal{I}}_0\}_0\}) + O(g^3)
\]

\[
= g^2 \langle \frac{1}{2}[\hat{S}_1, \hat{S}_0, \hat{A}] \rangle_0 + O(g^3)
\]

\[
= \langle \frac{1}{2}[\hat{S}, [\hat{S}, \hat{A}]] \rangle_0 + O(g^3)
\]

\[
= \langle \hat{A} \rangle_0 - \langle \hat{A} \rangle_0 + O(g^3)
\]

\[
= \langle \prod_{i=1}^m \tilde{\mathcal{I}}_{\alpha_i} \rangle_0 - \langle \prod_{i=1}^m \tilde{\mathcal{I}}_{\alpha_i} \rangle_0 + O(g^3)
\]

(D3)

In the second step we have used that \(\hat{H}_1\) involves only the creation and annihilation operators that occur in \(\hat{H}_0\) so that Wick’s theorem can be applied, yielding some function \(F\) of the occupation numbers, which are then related to initial-state expectation values in leading order in \(g\). Then \(F\) is eliminated by applying Wick’s theorem backwards. Finally, equating Eqs. (8) and (D1) yields the condition (20).