Typical Relaxation of Isolated Many-Body Systems Which Do Not Thermalize

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We consider isolated many-body quantum systems which do not thermalize; i.e., expectation values approach an (approximately) steady longtime limit which disagrees with the microcanonical prediction of equilibrium statistical mechanics. A general analytical theory is worked out for the typical temporal relaxation behavior in such cases. The main prerequisites are initial conditions which appreciably populate many energy levels and do not give rise to significant spatial inhomogeneities on macroscopic scales. The theory explains very well the experimental and numerical findings in a trapped-ion quantum simulator exhibiting many-body localization, in ultracold atomic gases, and in integrable hard-core boson and XXZ models.

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The long-standing task to explain macroscopic equilibration phenomena in terms of the underlying microscopic quantum dynamics is presently regaining considerable attention [1–3]. Since open systems are beyond the realm of standard quantum mechanics, the common starting point is an isolated many-body system, possibly incorporating the environment of the subsystem of actual interest. The question whether and how such a system or subsystem approaches some thermal or nonthermal equilibrium state after a sufficiently long time has been at the focus of numerous analytical [4–6], numerical [7–12], and experimental [13–18] studies. Despite the reversible and everlasting motion of the microscopic degrees of freedom, it could be shown in Refs. [19,20] under increasingly weak assumptions about the system Hamiltonian, the initial condition, and the considered observable that expectation values must remain extremely close to a constant value for the vast majority of all sufficiently late times (the exceptional times include initial transients and quantum revivals).

The natural next question is whether the system thermalizes, that is, whether the longtime behavior is well approximated by the pertinent microcanonical expectation value from equilibrium statistical mechanics. A first prominent criterion for thermalization is the so-called eigenstate thermalization hypothesis (ETH), postulating that every energy eigenstate yields expectation values close to the corresponding microcanonical values [5–8]. In other words, a violation of ETH is commonly considered an indicator of nonthermalization [1,6–9]. A related but different such indicator is the existence of additional conserved quantities (besides the system Hamiltonian) which can be written as sums of local operators, and which play a particularly prominent role for so-called integrable systems [1]. Numerically, it has been found that such systems usually violate the ETH and do not thermalize [7–9]. Instead, the longtime behavior is well captured by a so-called generalized Gibbs ensemble (GGE), which is obtained by the standard working recipe to maximize the von Neumann entropy under the constraints that the expectation values of the conserved quantities must be correctly reproduced [7]. Yet another common distinction between integrable and nonintegrable systems is the statistics of the gaps between neighboring energy levels E_n [1]. Further prominent examples which do not thermalize are systems exhibiting many-body localization (MBL) [2,11,12,16]. Compared to integrable systems, they are structurally more robust against small changes of the model Hamiltonian, but they otherwise seem to be quite similar, e.g., regarding energy level statistics, conserved quantities, ETH violation, and the GGE [1,2,21].

The objective of our Letter is a quantitative analytical description of the temporal relaxation in the absence of thermalization. Our approach is thus complementary to the numerical case studies, e.g., in Refs. [9,12,21,22]. Related analytical investigations are also quite numerous [20,23,24]. Yet, for each of them, a closer look at the considered systems and the obtained results reveals quite significant differences from our approach. For instance, some of them concern only thermalizing systems, others focus on special observables or on deriving upper and lower bounds for the temporal relaxation, etc. Particularly little is known about equilibration time scales in isolated systems which do not thermalize. Likewise, pertinent experimental works are still rather scarce [13–17]. A comparison of our theory with exemplary numerical and experimental results is provided later.

Going *in medias res*, let us consider a Hamiltonian H with eigenvalues E_n and eigenvectors $|n\rangle$ and an arbitrary initial state $\rho(0)$ (pure or mixed and, in general, far from equilibrium). According to textbook quantum mechanics, its temporal evolution is $\rho(t) = \mathcal{U}_t \rho(0) \mathcal{U}_t^\dagger$, with $\mathcal{U}_t := e^{-iHt/\hbar}$. Hence, the expectation value $\langle A \rangle_\rho := \mathrm{Tr}\{\rho A\}$ of an arbitrary observable A follows as

$$\langle A\rangle_{\rho(t)} = \sum_{m,n} \rho_{mn}(0) A_{nm} e^{i(E_n - E_m)t/\hbar}, \quad (1)$$

where $A_{mn} := \langle m|A|n\rangle$, $\rho_{mn}(t) := \langle m|\rho(t)|n\rangle$ and where, depending on the specific model under consideration, m and n run from 1 to infinity or to some finite upper limit. Averaging Eq. (1) over all $t \geq 0$ yields the result $\langle A\rangle_{\bar{\rho}}$, where the diagonal ensemble $\bar{\rho}$ is defined via $\bar{\rho}_{mn} := \delta_{mn}\rho_{nn}(0)$ [25]. Hence, if the system equilibrates at all, Eq. (1) must stay extremely close to $\langle A\rangle_{\bar{\rho}}$ for practically all sufficiently large t's (see above).

As usual, we focus on systems with a macroscopically well-defined energy; i.e., all energy levels E_n with non-negligible populations $\rho_{nn}(0)$ must be contained in an interval $I_E := [E-\epsilon, E]$ of macroscopically small (but microscopically large) width ϵ. Furthermore, we adopt the idealization that the probability $\rho_{nn}(0)$ to observe an energy E_n outside I_E can be approximated as strictly zero. The number of energies E_n contained in I_E is denoted by D and, without loss of generality, we assume that $n \in \{1, \ldots, D\}$ for all those E_n's. The Cauchy-Schwarz inequality $|\rho_{mn}|^2 \leq \rho_{mm}\rho_{nn}$ then implies that only $m, n \leq D$ actually matters in Eq. (1) and in all that follows. Specifically, the effectively relevant Hamiltonian is $H_1 := \sum_{n=1}^{D} E_n |n\rangle\langle n|$.

Denoting by π any permutation of $\{1, \ldots, D\}$, we define

$$H_\pi := \sum_{n=1}^{D} E_n |\pi(n)\rangle\langle\pi(n)| = \sum_{n=1}^{D} E_{\pi^{-1}(n)} |n\rangle\langle n|. \quad (2)$$

Hence, H_π is obtained by permuting either the eigenvalues or the eigenstates of the original Hamiltonian H_1.

In general, every H_π entails a different evolution of $\rho(t)$. Accordingly, in Eq. (1) either the energies or the matrix elements must be permuted analogously as in Eq. (2). On the other hand, one readily sees that the following important quantities and properties are invariant under arbitrary permutations π: (i) the energy spectrum, and hence the level statistics; (ii) the violation or nonviolation of the ETH; (iii) the conserved quantities [26]; (iv) the initial expectation value $\langle A\rangle_{\rho(0)}$. (v) for the vast majority of all sufficiently large t's, the expectation value $\langle A\rangle_{\rho(t)}$ stays extremely close to $\langle A\rangle_{\bar{\rho}}$, with the same diagonal ensemble $\bar{\rho}$ for all H_π's, and likewise for the GGE.

The main result of our Letter concerns the π and t dependent relaxation of $\langle A\rangle_{\rho(t)}$ and reads

$$\langle A\rangle_{\rho(t)} = \langle A\rangle_{\bar{\rho}} + F(t)\{\langle A\rangle_{\rho(0)} - \langle A\rangle_{\bar{\rho}}\} + \xi_\pi(t), \quad (3)$$

$$F(t) := \big(D|\phi(t)|^2 - 1\big)/(D-1), \quad (4)$$

$$\phi(t) := D^{-1} \sum_{n=1}^{D} e^{iE_n t/\hbar}. \quad (5)$$

The only π dependent term on the right-hand side of Eq. (3) is $\xi_\pi(t)$ and satisfies, for $D \geq 6$, the following key properties:

$$[\xi_\pi(t)]_\Pi = 0, \qquad [\xi_\pi^2(t)]_\Pi \leq (6\Delta_A)^2 \max_n \rho_{nn}(0), \quad (6)$$

where Π denotes the set of all permutations of $\{1, \ldots, D\}$ and $[\cdots]_\Pi$ the average over all $\pi \in \Pi$. Furthermore, Δ_A is the measurement range of the observable A, i.e., the difference between its largest and smallest eigenvalues.

Equations (3)–(6) are exact analytic results when $D \geq 6$ and for arbitrary H's, A's, and $\rho(0)$'s, with $\rho_{nn}(0) = 0$ for $n > D$. Their detailed mathematical derivation is quite tedious and provides very little physical insight; hence, it has been postponed to the Supplemental Material [27].

Since a typical many-body system exhibits an extremely dense energy spectrum (exponential in the degrees of freedom), it is practically impossible (e.g., in an experiment) to notably populate only a few energy levels; hence, $\max_n \rho_{nn}(0)$ must be unimaginably small [19]. Observing that $1/D \leq \max_n \rho_{nn}(0)$ implies that $D \gg 1$ in Eqs. (4) and (5), that the number $D!$ of permutations $\pi \in \Pi$ is gigantic, and that $[\xi_\pi^2(t)]_\Pi$ in Eq. (6) is exceedingly small. As a consequence, $\xi_\pi(t)$ itself must be very small for the vast majority of all $\pi \in \Pi$; i.e., we can safely approximate Eq. (3) by

$$\langle A\rangle_{\rho(t)} = \langle A\rangle_{\bar{\rho}} + F(t)\{\langle A\rangle_{\rho(0)} - \langle A\rangle_{\bar{\rho}}\}. \quad (7)$$

Specifically, this approximation also applies to the "true" system H_1, unless there are special reasons why its temporal relaxation should notably differ from that of practically all other H_π's.

A first very strong argument why the true system may be expected to exhibit the typical relaxation behavior (7) is the abovementioned invariances (i)–(v) under arbitrary permutations π. In fact, when considering the corresponding Hamiltonians H_π as a matrix ensemble, our situation is essentially just a particular instance of random matrix theory [28], whose predictions are well known to be surprisingly successful in many cases, provided that the ensemble preserves a few very basic properties of the true system of actual interest [28] [e.g., symmetries, or the invariances (i)–(v) in our case].

On the other hand, usual model Hamiltonians H_1 only involve short-range interactions (or local operators) [1,2], while most other H_π's do not preserve this "local structure." Spatial inhomogeneities of particle numbers, energy, etc. are thus expected to be balanced out increasingly slowly over increasing distances when H_1 governs the dynamics, but not for most other H_π's. Note that instead of permuting the energy eigenvectors $|n\rangle$ in Eq. (1) according to Eq. (2), one could replace $\rho(0)$ by $\rho_\pi(0) := U_\pi^\dagger \rho(0) U_\pi$, where the unitary U_π is defined via $U_\pi|n\rangle = |\pi(n)\rangle$ (and likewise for A, while H_1 is now kept fixed). Once again, even when

$\rho(0) = \rho_1(0)$ exhibits spatial inhomogeneities, one expects that most other $\rho_\pi(0)$'s will appear (nearly) homogeneous; hence, the local structure of H_1 yields an untypically slow relaxation of $\rho(0)$ [compared to most other $\rho_\pi(0)$'s]. In either case, it follows that our prediction (7) must be restricted to initial conditions without any significant spatial inhomogeneities on macroscopic scales.

A typicality result similar to Eqs. (3)–(6) was obtained by formally quite dissimilar methods in Ref. [24]. Conceptually, the essential difference is that arbitrary unitary (Haar distributed) basis transformations, rather than just eigenvector permutations in Eq. (2), were admitted in Ref. [24], resulting in the appearance of the microcanonical instead of the diagonal ensemble on the right-hand side of Eq. (3). In contrast to our work, the approach from Ref. [24] is thus restricted to systems which do thermalize. The main reason is that the permutations are a tiny subset (of measure zero) of all unitary basis transformations and thus may preserve additional key features of the true Hamiltonian H_1. For example, permutations preserve each of the above-mentioned properties (i)–(v), but general unitaries preserve only (i) and (iv). In return, the smallness of $\max_n \rho_{nn}(0)$ on the right-hand side of Eq. (6) is no longer required when admitting arbitrary unitaries [24]. In passing, we note that conditions similar to or even identical to $\max_n \rho_{nn}(0) \ll 1$ already arise in the general equilibration results from Refs. [19,20].

Turning to the function $F(t)$ in Eqs. (4) and (5), one readily sees that $F(0) = 1$ and $1 \geq F(t) > -1/D$ for all t's. Moreover, the following properties were derived previously in Ref. [24]: (i) $F(t)$ remains negligibly small for the vast majority of all sufficiently large t's, provided the maximal energy degeneracy is much smaller than D. (ii) Denoting by $\Omega(E)$ the number of energies E_n below E, by k_B and $S(E) = k_B \ln \Omega(E)$ Boltzmann's constant and entropy, respectively, and by $T := 1/S'(E)$ the corresponding formal temperature, one can often approximate the sum in Eq. (5) by an integral over a suitably smoothened level density, yielding the approximation

$$F(t) = 1/[1 + (tk_B T/\hbar)^2]. \tag{8}$$

Note that T and $S(E)$ could be identified with the usual temperature and entropy for a thermalized system, but they have no immediate physical meaning for nonthermalizing systems.

Besides integrability and MBL, yet another (quite trivial) reason for nonthermalization may be that the non-negligible level populations $\rho_{nn}(0)$ are not confined to a macroscopically small energy interval [see above Eq. (2)]. Incidentally, this case can also be readily included in our present theory, namely, by choosing D and the labels n so that $n \in \{1, \ldots, D\}$ if and only if $\rho_{nn}(0)$ is non-negligible. As a consequence, Eq. (8) is, in general, no longer valid, while all other findings remain essentially unchanged.

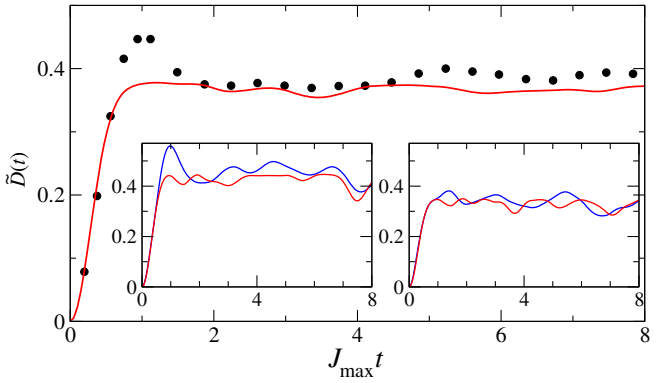

FIG. 1. (Symbols) The experimentally measured Hamming distance $\tilde{D}(t)$ from Fig. 3(a) of Ref. [16] for $W = 4J_{\max}$, averaged over 30 realizations of the disorder in Eq. (9). (Line) Corresponding theory from Eq. (7). (Insets) Theory (red curves) and numerical solutions (blue curves) for two representative realizations of the disorder in Eq. (9).

As a first example, we consider the experiment by Smith *et al.* [16] with $N = 10$ ions in a linear Paul trap, emulating the disordered Ising Hamiltonian

$$H = \sum_{i<j} J_{ij} \sigma_i^x \sigma_j^x + \frac{B}{2} \sum_i \sigma_i^z + \sum_i \frac{D_i}{2} \sigma_i^z \tag{9}$$

with $i, j = 1, \ldots, N$, the Pauli matrices $\sigma_i^{x,z}$, the couplings $J_{ij} = J_{\max}/|i-j|^{1.13}$, the homogeneous field $B = 4J_{\max}$, the uniformly distributed random fields $D_i \in [-W, W]$, and $\hbar = 1$. Initializing the spins in the Néel state $|\uparrow\downarrow\cdots\uparrow\downarrow\rangle$, the system exhibits MBL for disorder strengths beyond about $W = J_{\max}$ [16]. As was noted in Ref. [22], the experimentally measured Hamming distance $\tilde{D}(t)$ from Ref. [16] can be recovered as the expectation value of the observable $A := (1 - M)/2$ with $M := N^{-1} \sum_i (-1)^i \sigma_i^z$ (staggered magnetization).

In Fig. 1, the experimental results are compared with our theoretical approximation (7), (4) by introducing the numerically determined energies E_n of the Hamiltonian (9) into Eq. (5). Furthermore, as in the experiment, we averaged the so obtained results for $\tilde{D}(t)$ over 30 realizations of the disorder in Eq. (9). Since there are only $N = 10$ spins, $\max_n \rho_{nn}(0)$ is typically not yet very small and increases with W. We therefore focused on a moderate disorder of $W = 4J_{\max}$, and we considered labels n with $\rho_{nn}(0) < 0.01$ as negligible (see above), resulting in typical values $\max_n \rho_{nn}(0) \approx 0.1$ and $D \approx 20$. The concomitant approximations for $\langle A \rangle_{\rho(0)}$ turned out to exhibit particularly strong finite-N effects; hence, we used the *a priori* known actual value $\langle A \rangle_{\rho(0)} = 0$ in Eq. (7).

Besides those disorder averaged results, individual realizations of Eq. (9) would also seem interesting. Since experimental data are not available, we replicated the numerical solutions of the Schrödinger equation with

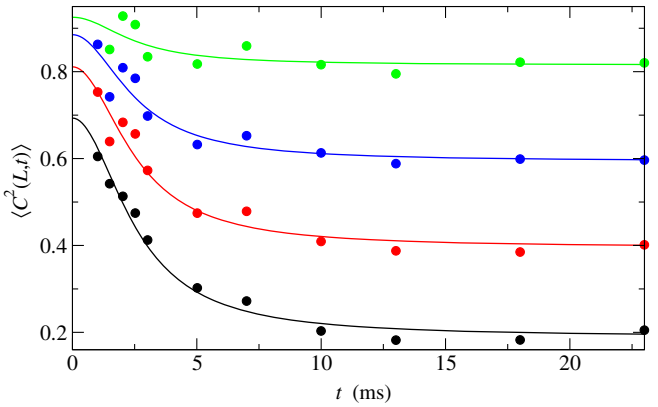

FIG. 2. (Symbols) Experimental mean integrated squared contrast from Fig. 3 in Ref. [14] for integration lengths $L = 18$, 40, 60, and 100 μm (from top to bottom) and vertically shifted by 0.3, 0.2, 0.1, and 0.0, respectively, for better visibility. (Lines) Theoretical approximation (7), (8) with $T = 3$ nK.

Hamiltonian (9) from Refs. [16,22]. The results for two realizations are shown in the insets of Fig. 1. The theoretical curves have been obtained as described above, employing the same realization of Eq. (9) as in the numerics in each inset. In view of those quite notable finite size fluctuations, the theory explains the "real" temporal relaxation remarkably well.

Next, we consider the equilibration of a coherently split Bose gas, as observed experimentally by Kuhnert *et al.* in Ref. [14] via the mean integrated squared contrast $\langle C^2(L,t)\rangle$ of the matter-wave interference pattern for various integration lengths L. This experiment (approximately) realizes an integrable system, exhibiting prethermalization rather than thermalization [13]. The data from Ref. [14] are compared in Fig. 2 with our theory Eq. (7). Since modeling the quite intricate observable of the actual experiment goes beyond our present scope, we treated $\langle A\rangle_{\rho(0)}$ and $\langle A\rangle_{\bar{\rho}}$ in Eq. (7) as fit parameters for any given L. Similarly, estimating the experimentally relevant "effective temperature" T in Eq. (8) from first principles is beyond our present scope; hence, it was treated as a fit parameter (common to all L's), yielding $T = 3$ nK. In fact, Fig. 5 in Ref. [15] suggests that the experimental estimate $T_{\text{eff}} \approx 10 \pm 3$ nK from Fig. 2 (at $t_e = 0$ ms) in Ref. [13] may also be a reasonable approximation in our present case. Here, T_{eff} is yet another effective temperature which would agree with T at thermal equilibrium, but may well be different from T in our case. Furthermore, the experimental estimate of T_{eff} is based on a quite involved procedure [13] whose implicit premises may only be approximately satisfied. In conclusion, $T = 3$ nK seems still compatible with the experimental findings, and the resulting theoretical curves in Fig. 2 explain the main features of the data quite well.

As a third example, we turn to the numerical results for an integrable model by Rigol [9], consisting of eight hard-core bosons on a periodic one-dimensional lattice with 24 sites, and exhibiting nonthermal longtime expectation values. The detailed definition of the considered observable $\delta n_k(t)$ from Ref. [9] is not repeated here since only the initial and longtime values are actually needed in Eq. (7), whose quantitative values cannot be estimated theoretically anyway and hence are treated as fit parameters. Furthermore, we adopted the approximation (8) with the estimate $T = 2$ from Ref. [9] (in units where $k_B = \hbar = 1$). The resulting agreement with the numerical data in Fig. 3 is remarkably good, considering that the system consists of just eight bosons.

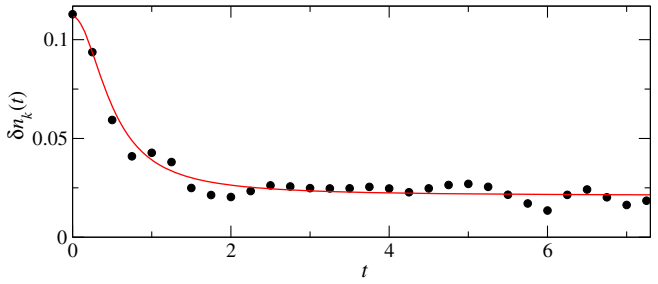

FIG. 3. (Symbols) Numerical results from Fig. 1(e) of Ref. [9]. (Line) Theoretical approximation (7), (8). For further details, see the text.

Our last example is the integrable XXZ model of Torres-Herrera *et al.* from Ref. [29]. Similarly as before, the initial value $\langle A\rangle_{\rho(0)} = 0.25$ in Eq. (7) is known *a priori* for the specific observable under consideration, while $\langle A\rangle_{\bar{\rho}}$ is treated as a fit parameter. On the other hand, $F(t)$ is now evaluated via Eq. (4) by approximating the discrete levels on the right-hand side of Eq. (5) by a continuous level density [24]. In view of Table 1 and Fig. 3(b) in Ref. [29], we roughly approximated this density as constant within the energy interval $I_E = [-1.8, 1.8]$, and as zero otherwise. The resulting agreement with the numerics in Fig. 4 speaks for itself.

In conclusion, we devise in this Letter a general analytical theory for the temporal relaxation behavior of isolated many-body systems which do not thermalize. The

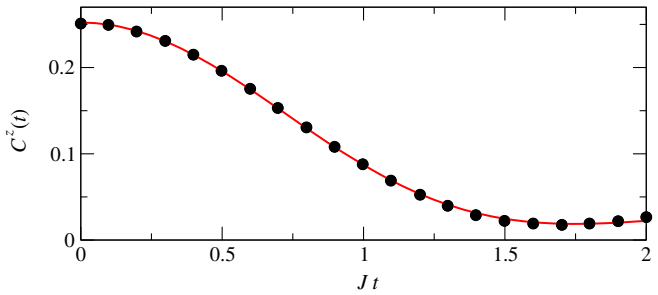

FIG. 4. (Symbols) Numerical results for the spin-spin correlation $C^z(t)$ from Fig. 8 of Ref. [29] for a spin-1/2 XXZ model with 16 spins, coupling J, anisotropy $\Delta = 1/2$, $\hbar = 1$, and a so-called pairs of parallel spins initial condition. (Line) Theoretical approximation (7), as specified in the text.

main prerequisites are initial conditions which appreciably populate many energy levels and do not give rise to significant spatial inhomogeneities on macroscopic scales. Specifically, the relaxation must not entail any significant transport currents, caused by some unbalanced local densities (of particles, energy, etc.). On the other hand, the particular reason for the absence of thermalization (MBL, integrability, broad energy distribution) seems largely irrelevant. In fact, our theory also applies to systems which do thermalize, provided that the diagonal and microcanonical ensembles yield identical expectation values due to, e.g., the validity of the ETH. Compared to previous related studies, our main new concept consists in admitting only permutations of basis vectors in Eq. (2), rather than arbitrary (Haar distributed) basis transformations, thus preserving all local constants of motion, the diagonal ensemble which governs the longtime behavior, and the violation (or not) of the ETH. The adequate treatment of inhomogeneous initial conditions remains an important challenge for future research.

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[25] If H exhibits degeneracies, we tacitly choose the eigenvectors $|n\rangle$ so that $\rho_{mn}(0)$ is diagonal within every eigenspace.

[26] Any conserved quantity C satisfies $[C, H_1] = 0$ and thus implies a common eigenbasis of C and H_1. For a nondegenerate H_1, this basis must be $\{|n\rangle\}_{n=1}^{D}$, and with Eq. (2), it follows that $[C, H_\pi] = 0$. If H_1 exhibits degeneracies, H_π still possesses just as many conserved quantities as H_1, but, in general, they are no longer identical.

[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.118.190601 for the derivation of Eqs. (3)–(6).

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