

BREAKING OF QUANTUM ERGODICITY AND SCARS

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In this article quantum chaos is introduced, with special attention to the concept of ergodicity, and compared to classical counterparts. The eigenstate thermalization hypothesis, a statement of ergodicity in quantum mechanics, is discussed. Methods of breaking ergodicity by way of violating the hypothesis are discussed. These are separated into strong breaking, including integrability and many-body localization, and weak breaking, notably including many-body scars and related effects.

ZLOM KVANTNE ERGODIČNOSTI IN BRAZGOTINE

V članku je uveden kvantni kaos ter primerjan s klasičnim, s poudarkom na pojmu ergodičnosti. Hipoteza o termalizaciji lastnih stanj (ang. *eigenstate thermalization hypothesis*), ki deluje kot ustreznica ergodičnosti v kvantni mehaniki, je predstavljena. Sledi razprava o nekaterih načinih zloma ergodičnosti preko zloma omenjene hipoteze. Ti so ločeni na močan zlom, ki ga povzročita integrabilnost in mnogodelčna lokalizacija (ang. *many-body localization*), in šibak zlom, ki ga povzročijo mnogodelčne kvantne brazgotine (ang. *many-body quantum scars*) ter sorodni učinki.

1. Introduction

To study quantum chaos, we must consider a system out of equilibrium that is governed by the laws of quantum mechanics. To push the system out of equilibrium, we rapidly change some parameter, e.g. by applying an electromagnetic field, after which we observe the so-called quench process. This is of particular interest to us along this article. We look at closed interacting many-body quantum systems, that is systems of many, sometimes quite strongly, interacting constituent parts (i.e. particles). These systems do not exchange energy with the environment and therefore evolve only due to their own Schrödinger's equation.

2. Quantum chaos

Because quantum-mechanical position and momentum do not commute, phase diagrams of their trajectories are essentially infeasible. Despite this, we can find counterparts of classical chaos theory in quantum mechanics. Wavefunctions, eigenvalues and eigenstates can behave periodically, i.e., propagate back to their origin, or be stable with respect to perturbation. The correspondence principle further motivates us to expect that quantum counterparts of classically chaotic systems should show high sensitivity to initial conditions and otherwise behave analogously [1].

Another important concept related to chaos theory is *ergodicity* – the property of a dynamical system whose time average is synonymous with its phase-space average. The phase space of a classical ergodic system is then (evenly) covered by the trajectory of some point evolving in time. In further sections, we attempt to define a quantum counterpart to classical ergodicity, such that its intuitive description is somewhat preserved. Properties of chaos and ergodicity are illustrated in Fig. 1.

After a transient period, a state out of equilibrium will generally evolve into equilibrium. If this process is predicted by statistical mechanics and expectation values of observables in the resulting equilibrium obey the canonical or microcanonical ensemble, the process is called thermalization and is irreversible [3]. A non-thermal equilibrium can also be reached, where the system's observables

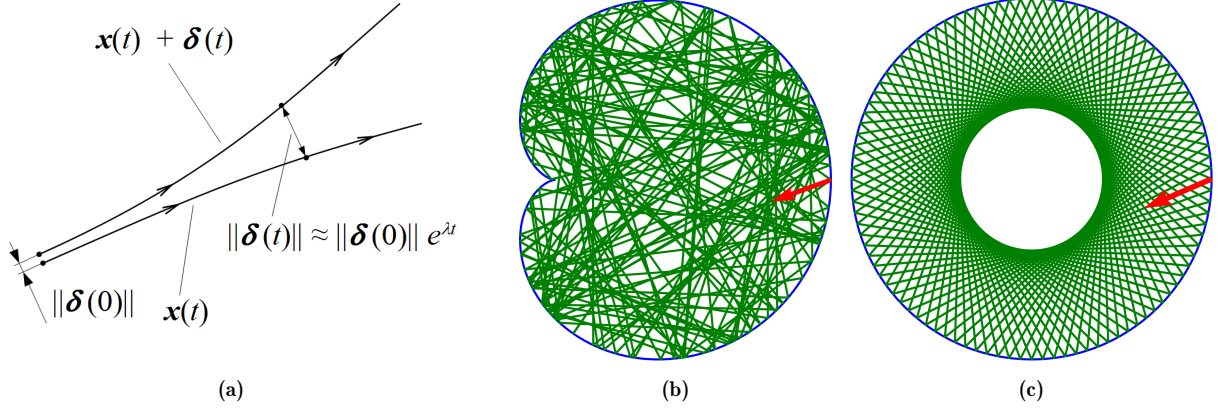


Figure 1. (a) The distance $\|\delta(t)\|$ between two trajectories that were initially close together can be described by the so-called Lyapunov exponent λ . Informally speaking, when this exponent is larger than 0, the system is behaving chaotically. (b) A cardioid billiard, a dynamical system of particles elastically colliding with a cardioid-shaped boundary, exhibits ergodic behaviour as typical trajectories are seen to fill the phase space evenly. (c) A disk billiard, on the other hand, is non-ergodic, as trajectories typically miss some large part of the phase space, e.g., the center. Panel a reproduced from Ref. [2].

are not described by either of these ensembles (see, e.g., Fig. 1 and accompanying text in Ref. [4]).

An important sidenote: A chaotic system is not necessarily an ergodic one, and vice-versa – the former is characterized by the high rate at which two typical initially close trajectories separate, which does not necessitate them exploring the phase space evenly. Large systems, with many degrees of freedom, are generally chaotic and ergodic [5].

2.1 Ergodicity according to von Neumann

We explore a short derivation which roughly outlines how we can at first blush relate classical to quantum ergodicity. First, the classical case: Consider an initial state X_0 at energy E , which evolves to be $X(t)$ after some time t . What follows for a classical ergodic system is that by long-time averaging, we can get the state density for some state X

$$\overline{\delta[X - X(t)]} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \delta[X - X(t)] dt \stackrel{\text{ergodicity}}{=} \rho_{\text{mc}}(X, E), \quad (1)$$

where $\delta[X - X(t)]$ equals one at times t when X and $X(t)$ are equal (overlap) and zero otherwise. The integral in Eq. (1) can therefore be interpreted as counting up all the states that find themselves at X . Ergodicity also ensures that some typical (random) choice of X_0 is enough to probe the entire phase space, and that (almost) any such choice is good enough. By calculating $\rho_{\text{mc}}(X, E)$ at all possible X , we have obtained the state density of the *microcanonical ensemble* – a well-studied concept in statistical mechanics.

For a quantum system, the analogue can be written as an operator

$$\hat{\rho}_{\text{mc}}(E) = \sum_{\alpha} \frac{1}{N} |\psi_{\alpha}\rangle \langle \psi_{\alpha}|, \quad (2)$$

where we sum over all α whose states $|\psi_{\alpha}\rangle$ are part of the energy shell $[E, E + \delta E]$. Here N is the number of all such states, and each state is represented with equal probability $1/N$. For an ergodic system, we should expect an analogue of Eq. (1) to hold true, so we write

$$\overline{|\psi(t)\rangle \langle \psi(t)|} = \hat{\rho}(E), \quad (3)$$

where we wrote the evolution of $|\psi(0)\rangle = \sum_{\alpha} c_{\alpha} |E_{\alpha}\rangle$, where $c_{\alpha} = \langle E_{\alpha}|\psi(0)\rangle$, as

$$|\psi(t)\rangle = \sum_{\alpha} e^{-iE_{\alpha}t} c_{\alpha} |E_{\alpha}\rangle = \left(\sum_{\alpha} e^{-iE_{\alpha}t} |E_{\alpha}\rangle \langle E_{\alpha}| \right) |\psi(0)\rangle. \quad (4)$$

Now we evaluate Eq. (3) using Eq. (4) while assuming a non-degenerate system (no states with duplicate energies). This gives $\sum_{\alpha} |c_{\alpha}|^2 |\psi_{\alpha}\rangle \langle \psi_{\alpha}|$, which must equal Eq. (2), so we conclude that

$$|c_{\alpha}|^2 = 1/N \quad (5)$$

for all α , which is of course not always true. We can define a „diagonal“ ensemble

$$\hat{\rho}_{\text{diag}} = \sum_{\alpha} |c_{\alpha}|^2 |\psi_{\alpha}\rangle \langle \psi_{\alpha}| \quad (6)$$

so Eq. (5) in essence requires that $\hat{\rho}_{\text{diag}} = \hat{\rho}_{\text{mc}}$ [6, 7]. The general construction of the diagonal ensemble in Eq. (6) would otherwise allow a dependence on the initial state coefficients c_{α} , which would be at odds with ergodicity, as information about the initial state would not get lost during time evolution.

Quantum ergodic systems, as required by Eqs. 5 and 6, are very rare. This derivation is a part of John von Neumann’s work from 1929 [8], where he noted that we can also shift our focus from states to observables with the requirement (without derivation)

$$\overline{\langle \psi(t) | \hat{A}_{\alpha}(t) | \psi(t) \rangle} = \text{Tr}\{\hat{A}_{\alpha} \hat{\rho}_{\text{diag}}\},$$

which should hold for almost all observables $\hat{A}_{\alpha}$ and initial conditions, a similar but easier to satisfy condition than Eq. (5) [7].

2.2 Eigenstate thermalization hypothesis

By shifting our focus away from states entirely, we can formulate one important definition of ergodicity in quantum mechanics: The so-called *eigenstate thermalization hypothesis* (ETH). Though the ETH is a statement of thermalization, not quantum ergodicity, equivalence between the two is usually assumed and has also been shown rigorously [9]. To construct the hypothesis, we consider a matrix element of some observable A in energy eigenstates $|E_{\alpha}\rangle$ and $|E_{\beta}\rangle$, i.e. $\langle E_{\alpha} | A | E_{\beta} \rangle$. The diagonal elements ($\alpha = \beta$), sorted by energy, should not be far apart from each other or change quickly with the state, neither should the non-diagonal elements ($\alpha \neq \beta$) be themselves too big (w.r.t. system size). If these statements are true, the expected value of A tends to an equilibrium value predicted by the microcanonical ensemble, i.e., thermalizes for any choice of initial pure state [10]. If almost all of the diagonal elements (eigenstates) follow the ETH and only a small fraction violates it, we say the system follows the weak ETH and breaks ergodicity weakly [5].

The ETH can then be less formally understood as requiring expectation values to change with energy eigenstates smoothly, the energy spectrum being without bumps, and afterwards stating that thermalization happens, for all eigenstates whose diagonal elements obey this requirement. Diagonal matrix elements being close to each other (or practically equal) in value also corresponds to the ensemble being microcanonical, which is something that can also be intuited from Eq. (5) [7]. Another possible formulation of the hypothesis states that the expectation value $\langle E_{\alpha} | A | E_{\alpha} \rangle$ is equal to the average (arithmetic mean) over all expectation values within the same energy band, that is close in energy to E_{α} , which also evokes microcanonicity. This condition is analogous to the one of smooth transitions in diagonal elements mentioned above [11].

Though the choice of A is essentially arbitrary, and we can always construct operators for which the ETH holds, it's most useful to choose physically relevant (measurable) observables. While the ETH has been numerically verified plenty of times, no analytical proof exists yet. It is therefore not entirely clear if all thermalization can be explained by the ETH, or if there may be other alternative explanations, as not all states can be prepared experimentally – and some exotic states may yet exist which thermalize, but still violate the hypothesis. [5] Another caveat is that it does not say anything about the time scale of the process – for how long we have to average in Eq. (3) – only whether the system reaches thermal equilibrium or not [5].

3. Strong ergodicity breaking

We divide effects which prevent thermalization into strong and weak based on the degree to which they violate the ETH. Strong breaking violates the ETH in its entirety, so for most (if not all) eigenstates, which we explore below.

3.1 Integrability

When a system has an extensive number of conserved quantities, or constants of motion, they prevent it from thermalizing completely, and ergodicity is broken by *integrability* [7, 12].

In analogy with classical dynamical systems, the system can then be described in fewer dimensions than the phase space, i.e., on a submanifold. More formally, integrable Hamiltonian systems are defined as obeying Liouville integrability, which requires that conserved quantities are functionally independent from the Hamiltonian and from each other, and so a system with n degrees of freedom and a $2n$ -dimensional phase space has n conserved quantities (integrals of motion), with the condition that

$$\{F_i, F_j\} = 0 \quad \text{for } i, j = 1, 2, \dots, n.$$

Here $\{\bullet, \bullet\}$ denotes the Poisson bracket and F_i are functions of canonical coordinates $q_1, \dots, q_n$ and $p_1, \dots, p_n$, one of them being the Hamiltonian. The Liouville theorem then states that such a system is exactly solvable, i.e. the Hamiltonian equations of motion (differential equations) can be solved and the system's dynamics determined [13]. We can construct a quantum counterpart of this theorem by replacing the Poisson brackets with commutators and F_i with operators, therefore requiring that extensively many operators commute [13, 14].

In general, quantum many-body systems behave chaotically when integrability is broken, which can be achieved by applying a weak perturbation to an otherwise integrable system.¹ Ergodicity and the ETH are consequently also restored [7].

3.2 Many-body localization

A strong violation of the ETH can also occur through the mechanism of *many-body localization* (MBL) – a phenomenon caused by strong disorder, resulting in so-called emergent integrability and local conservation laws. MBL is strongly resistant to perturbation, in contrast with integrability's fragility. [15]

An example of MBL arising is the Heisenberg XXX model, a one-dimensional chain of N half-spin particles with the Hamiltonian

$$H = \sum_i^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z) - \sum_i^N h_i \sigma_i^z,$$

¹Integrability is unstable under perturbation, so while in the classical sense some features of orbits survive small perturbations due to the KAM theorem, quantum systems have no such equivalent formulation, and so quantum integrability requires fine-tuning to persist [12, 15].

where $\sigma_i^{x,y,z}$ are Pauli matrices and h_i is the strength of an outside magnetic field acting on the i -th particle.² This is an interacting model, and we can roughly consider two regimes: An ETH-abiding, thermalizing phase when h is low, and an ergodicity-breaking phase when h is high – the classical limit of particles in a magnetic field. During the transition from the former to the latter, inter-particle interaction weakens and in the wake of rising h eventually vanishes. This „disorder“ can therefore be seen to produce a system where energy may not flow between particles (i.e. suppressed diffusion) as they isolate from each other and behave locally in space, making thermalization impossible [4, 16].

What is perhaps most surprising is that this occurs at finite disorder, with some interaction still intact. The border between the ETH and non-ETH phases, called the many-body mobility edge, which appears (see Fig. 2) to depend on the distance between ground and maximum energy, called the energy density, which further depends on the system size [4].

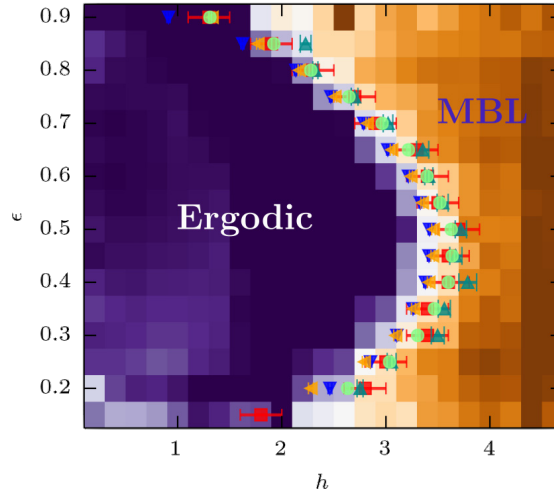


Figure 2. Critical disorder (many-body mobility edge) of the quantum phase transition between the ergodic (purple) and non-ergodic (orange) phases of a Heisenberg chain, simulated at different energy densities. Reproduced with permission from Fig. 1 in Ref. [17].

MBL breaks ergodicity by giving host to local integrals of motion, whose conservation prevents thermalization in a similar fashion to integrability, but in this case for local (not global) observables [18]. In practice, it is possible to completely diagonalize the system Hamiltonian, by first applying a unitary transformation to H , obtained from e.g. perturbing the high-disorder ($h \rightarrow \infty$) or late-time ($t \rightarrow \infty$) limits [4].

A related effect that largely predates the discovery of MBL is Anderson localization, which shares many phenomenological features with the former. Anderson localization describes how, in a system of a single particle that can tunnel between neighbouring spaces on a lattice, heightened disorder localizes the particle’s wavefunction on a single space and prevents it from further hopping – an effect that can, for example, explain the fall in conductance of (diffusion within) materials with impurities, a so-called Anderson isolator [19, 20].

MBL can then be viewed as a conceptual continuation of Anderson’s by adding interaction, though they are still separate phenomena and can occur one without the other or simultaneously [21]. Despite them being difficult to reliably discern experimentally, MBL largely differs because emergent local integrals of motion couple with each other and slowly dephase the system, whereas in Anderson’s localization the dephasing is quickly saturated [4, 22].

²When the magnetic field is homogenous ($h_i \equiv h$), the system becomes integrable, regardless of field strength h .

4. Weak ergodicity breaking and scars

Some systems follow only weak ETH, which can be caused by *quantum many-body scars* (QMBS). They represent a small (fraction zero of all eigenstates) quantity of highly excited non-thermal eigenstates in a spectrum of otherwise thermal eigenstates. Though they are few and far between, these ETH-violating eigenstates enable some very specific initial conditions to exhibit non-thermal dynamics [12].

QMBS get their name from single-particle quantum scars, which are also an interesting visualization of classical-quantum correspondence. Most demonstrably, we can consider a Bunimovich stadium billiard, a classically chaotic and ergodic system. When we propagate a Gaussian wavepacket through it semiclassically, some energy eigenstates $|\psi\rangle$ have their probability densities $|\psi|^2$ (or projections on test states, e.g., the original wavepacket) visibly increased in some areas of phase space. If these coincide with classical *unstable* periodic orbits in the stadium, the areas are termed (quantum) scars – see example in Fig. 3 [15, 23, 24].

Probability enhancement of scars is inversely proportional to the product between an orbit's Lyapunov (instability) exponent and period length, with stronger enhancements occurring when this product is far below and vanishing when equal to 1 [25]. This product can be understood as the spread of a wavepacket after it travels for one period, i.e., propagates back to its origin. Therefore, when a wavepacket spreads considerably, scars become less visible.

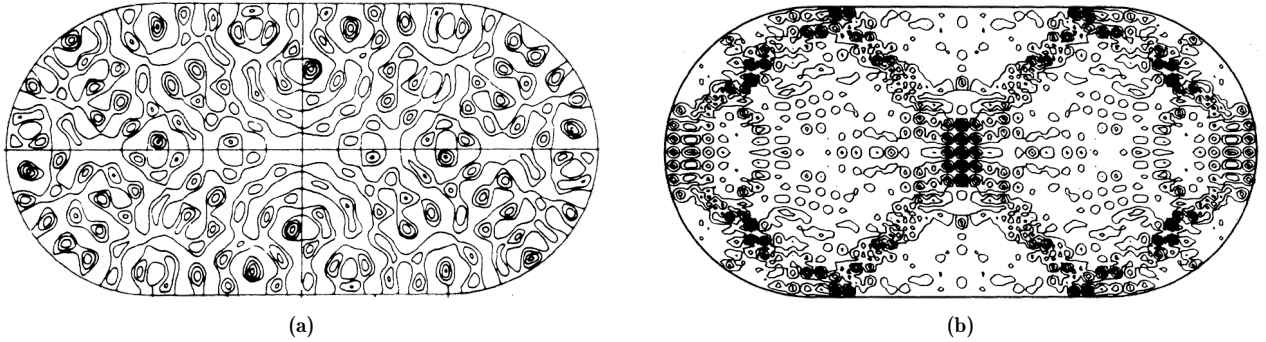


Figure 3. Contours of probability density $|\psi|^2$ of some eigenstates $|\psi\rangle$ for a Gaussian wavepacket in a Bunimovich stadium. (a) In contrast with a typical eigenstate, (b) a scarred eigenstate has enhanced probability density around an unstable period-6 orbit. Reproduced with permission from Ref. [24].

Though areas around classical stable periodic orbits are also enhanced, this is to be expected from classical systems, as stability implies multiple trajectories in a tight volume, whereas unstable orbits are extremely sparse in phase space, and should therefore cause no enhancement, making the quantum case unique [23].

An illustrative realization of QMBS is a chain of N Rydberg atoms – neutral atoms that may shift between the ground state $|\circ\rangle$ and a particular excited state $|\bullet\rangle$. When illuminated, they exhibit Rabi oscillations, jumping between the two states [15]. If the distance between the atoms is small enough, the van der Waals force prevents more than one neighbouring atom from being excited, prohibiting $|\dots\bullet\bullet\dots\rangle$ configurations. This regime is called the Rydberg blockade [26]. A model describing a Rydberg chain in the nearest-neighbour interaction limit is the effective PXP model, with the Hamiltonian

$$H = \sum_i^N P_{i-1} \sigma_i^x P_{i+1}, \quad (7)$$

where $\sigma_i^x = |\circ\rangle_i \langle\bullet|_i + |\bullet\rangle_i \langle\circ|_i$ is a Pauli matrix and $P_i = |\circ\rangle_i \langle\circ|_i$ a projector onto the ground state [14].

This model generally thermalizes, though there are some notable initial states whose eigenstates do not all follow the ETH, with even the ones that do doing so more slowly than expected [14]. In particular, quenches from initial states

$$|\mathbb{Z}_2\rangle = |\bullet \circ \bullet \circ \bullet \circ \bullet \dots\rangle \quad \text{and} \quad |\mathbb{Z}_3\rangle = |\bullet \circ \circ \bullet \circ \circ \bullet \dots\rangle \quad (8)$$

have been extensively explored. They are called the period-2 (or Néel) and period-3 density-wave states, respectively.³ [15]

After quenching from the states of Eq. (8), the non-thermal eigenstates manifest as towers (spikes) in the sea of thermal states, as seen in Fig. 4. In this case, evenly spaced towers are produced. Even though these violating eigenstates are sparse, ETH-violating periodic revivals of domain-wall density can be seen (see Fig. 6b at Ref. [26]), where the value keeps oscillating for a non-thermally long time with a frequency that depends on the energy spacing between the towers [14]. In other models, QMBS can also appear in isolation, and as there is no repeating structure, these cause no revivals in observables [12].

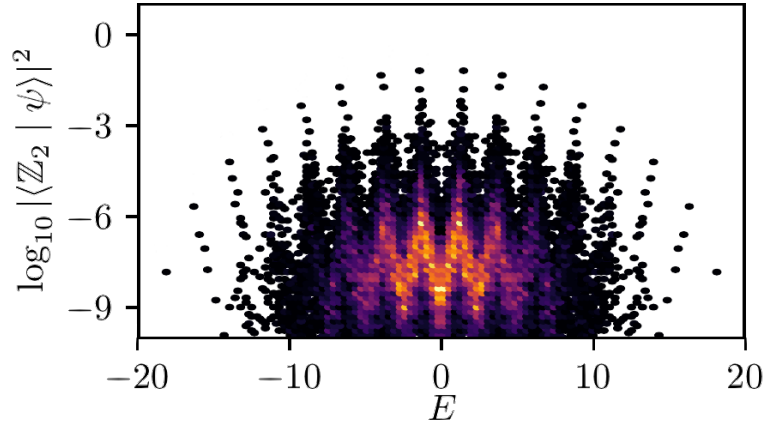


Figure 4. Evenly-spaced towers that cause revivals of the period-2 density-wave initial state (see Eq. (8)) in the PXP model. Quenched eigenstates overlap with the initial state at evenly spaced energies (color represents density). This spacing manifests itself in long-lived periodic revivals of the density of domain walls – neighbours that are either $|\circ\circ\rangle$ or $|\bullet\bullet\rangle$ (see Fig. 6b at Ref. [26]). Reproduced with permission from Ref. [14].

A common feature of QMBS is that Hilbert space can be viewed as approximately decoupled, and the Hamiltonian written in a block-diagonal form of scarred (non-thermal) and thermal components

$$H \approx H_{\text{scar}} \oplus H_{\text{thermal}}. \quad (9)$$

The scarred subspace does not necessarily host any symmetries to exist [15].

We can outline some general categories for the decoupling of Eq. (9). One is by a spectrum-generating algebra, where a local scar creation operator $\hat{Q}^+$ is defined, producing equally spaced energy eigenvalues of H_{scar} called towers [12, 15]. Another source of decoupling is Krylov restricted thermalization, which is described by constructing Krylov subspaces ending at some finite n : $\text{Span}\{|\psi\rangle, H|\psi\rangle, \dots, H^n|\psi\rangle\}$. These then constrain $|\psi\rangle$ from leaving its subspace of origin, effectively „restricting“ thermalization to it and allowing some other (decoupled) subspace to be non-thermalizing [15]. Finally and most generally, the mechanism of projector embedding attempts to merge a non-thermalizing subspace with a thermalizing one, by way of effectively projecting the former onto the latter [15].

³Weak ergodicity breaking seems to strongly depend on the choice of initial state, in contrast with strong breaking discussed in Sec. 3[14].

The PXP model described by Eq. (7) is a physical realization of spectrum-generating algebras, owing to its production of evenly-spaced towers, but it can also be interpreted from the other two mechanisms [14, 15].

5. Conclusions

Though quantum systems cannot be discussed in terms of strict trajectories, features of chaos can still be demonstrated. An important concept is the eigenstate thermalization hypothesis (ETH), which, when the conditions are met, states that a system's eigenstates and eigenvalues obey a thermal distribution and thus constitute an ergodic system.

There are many ways to „break“ ergodicity and violate the ETH, i.e., prevent a system from thermalizing. The degree to which ergodicity is broken is measured by how many eigenstates still follow the ETH.

Strong ergodicity is broken when no eigenstate thermalizes. This occurs if the system is integrable (i.e. has extensively-many conserved quantities) or is many-body localized (i.e. prohibits transport due to strong disorder).

Ergodicity can also be broken in the weak sense, where only a vanishingly small fraction of all eigenstates don't thermalize. This can be caused by quantum many-body scars (QMBS), an interacting many-body version of single-particle quantum scars. The latter appear as areas of increased probability density of some initial states around corresponding classical unstable periodic orbits, an effect classically sensible only for stable periodic orbits. One many-body scarred system is the one-dimensional PXP model of Rydberg atoms. Its scar-originating evenly-spaced excited states (towers) in the otherwise thermal spectrum coincide with periodical revivals of some observables, such as domain-wall density. QMBS can be theoretically explained as a decoupling of Hilbert space, owing to various possible mechanisms.

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