Chaos and Statistical Relaxation in Quantum Systems of Interacting Particles

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We study the transition to chaos and the emergence of statistical relaxation in isolated dynamical quantum systems of interacting particles. Our approach is based on the concept of delocalization of the eigenstates in the energy shell, controlled by the Gaussian form of the strength function. We show that, although the fluctuations of the energy levels in integrable and nonintegrable systems are different, the global properties of the eigenstates are quite similar, provided the interaction between particles exceeds some critical value. In this case, the statistical relaxation of the systems is comparable, irrespective of whether or not they are integrable. The numerical data for the quench dynamics manifest excellent agreement with analytical predictions of the theory developed for systems of two-body interactions with a completely random character.

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Introduction.—Recent experimental progress in the study of various quantum systems of interacting particles (see, e.g., [1]) has triggered interest in basic problems of many-body physics. One of the important issues is the onset of thermalization in isolated dynamical quantum systems due to interparticle interactions.

A prerequisite for thermalization is the statistical relaxation of the system to some kind of equilibrium and its viability has been associated with the onset of quantum chaos. The latter term was originally created to address specific properties of dynamical quantum systems whose classical counterparts are chaotic. Later, it was found that similar properties of spectra, eigenstates, and dynamics could emerge in quantum systems without a classical limit, as well as in quantum systems with disordered potentials. Nowadays, the term quantum chaos is used in a broader context when referring to those properties, irrespective of the existence of a classical limit.

According to studies of isolated quantum many-body systems, their eigenfunctions (EFs) in the mean-field (mf) basis spread as the interaction between particles (or quasiparticles) increases and they may eventually become chaotic eigenstates. The latter term refers to eigenstates with a large number of uncorrelated components, thus allowing one to use statistical methods for their description [2]. Examples based on experimental data include excited states of the cerium atom [3] and compound states in heavy nuclei [4].

It should be stressed that in isolated systems with finite-range interaction, only part of the basis states $|n\rangle$ defined by the noninteracting (quasi)particles is directly coupled when the perturbation is turned on. Thus, the exact eigenstates $|\alpha\rangle = \sum_n C_n^\alpha |n\rangle$ overlap only with some of the basis states, that is only a fraction of the components C_n^α can be nonzero. In the energy representation, this fraction constitutes the energy shell of the system. The definitions of localization, sparsity, and ergodicity that we use are made with respect to the energy shell [5]. The eigenstate is localized if its nonzero C_n^α's are restricted to a small portion of the shell. The eigenstate is delocalized if its nonzero components spread through the whole shell. In this last case, $|\alpha\rangle$ is either sparse, if not all components are nonzero, or ergodic, when it fills the shell entirely. Both show a very large number of principal components ($N_{\rm pc} \gg 1$) strongly fluctuating with n, but only the latter can lead to truly chaotic eigenstates. In chaotic eigenstates the coefficients C_n^α are random variables following a Gaussian distribution around the "envelope" defined by the energy shell. They occur when the interaction exceeds a critical value [2,5–7].

The energy shell is associated with the limiting form of the strength function (SF) written in the energy representation [5]. This function is defined via the projection of unperturbed states onto the basis of perturbed (exact) eigenstates. SF is widely used in nuclear physics and is analogous to the local density of states in solid state physics. It has been shown that the shape of SF changes from a Breit-Wigner (Lorentzian) to a Gaussian form as the interparticle interaction increases [2,6,8,9].

If a quantum system has a classical limit, the shapes of both EFs and SFs in the energy representation have classical analogs. The quantum-classical correspondence of EFs and SFs has been studied for various few and many-body systems (see Refs. [10,11]). Typically, delocalization of EFs in the energy shell is directly related to the chaotization of the system in the classical limit, thus providing a tool to reveal the transition to quantum chaos.

The emergence of chaotic eigenstates has been related to the onset of thermalization in many-body systems, even if the latter are isolated from a heat bath [2,6,7,11–16]. It was shown in [2,7,13] that when the eigenstates become chaotic, the distribution of occupation numbers achieves a Fermi-Dirac or a Bose-Einstein form, thus allowing for the introduction of temperature. Using a two-body random matrix model, a relation between temperature and interaction strength was analytically derived [2], implying that the interparticle interaction plays the role of a heat bath. Since the components of chaotic eigenstates can be treated as random variables, the eigenstates close in energy are statistically similar. This fact is at the heart of the eigenstate thermalization hypothesis [12], according to which the expectation values of few-body observables obtained with individual eigenstates correspond to the predictions from a microcanonical ensemble [14,15].

Even though works about the chaotization of eigenstates and its relevance to the problem of thermalization exist, they are mainly numerical, thus leaving various questions open. One of these problems, addressed in this Letter, is the analysis of generic conditions under which chaotic eigenstates emerge in dynamical systems of current interest in experiments with optical lattices. We consider systems of interacting spin-1/2 particles, but the results are equivalently valid to systems of spinless fermions or hard-core bosons. We propose a semianalytical method to estimate the critical interaction strength leading to the emergence of chaoticlike eigenstates, which does not require the diagonalization of the Hamiltonian matrices. We also show how this transition is reflected by the form of the strength functions. Another main goal of our work is the analytical description of the relaxation process of such dynamical systems, a problem that has not been sufficiently studied yet.

The models.—We consider two models of interacting spins-1/2. One model has only nearest-neighbor (NN) couplings which results in its complete integrability. The other model has additional next-nearest-neighbor (NNN) couplings and becomes chaotic when the two coupling strengths are comparable. Assuming open boundary conditions, the Hamiltonians read as

$$H_1 = H_0 + \mu V_1, \qquad H_2 = H_1 + \lambda V_2,$$
$$H_0 = J \sum_{i=1}^{L-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y), \qquad V_1 = J \sum_{i=1}^{L-1} S_i^z S_{i+1}^z,$$
$$V_2 = \sum_{i=1}^{L-2} J[(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y) + \mu S_i^z S_{i+2}^z], \tag{1}$$

where μ and λ control the perturbation in model 1 and model 2, respectively. Here, L is the number of sites, $S_i^{x,y,z} = \sigma_i^{x,y,z}/2$ are the spin operators at site i, with $\sigma_i^{x,y,z}$ as the Pauli matrices and $\hbar = 1$. The coupling strength J defines the energy scale and is set to 1.

In model 1, H_0 determines the mf basis in which the total Hamiltonian H_1 is presented. This term moves the up spins through the chain and can be mapped onto a system of noninteracting spinless fermions [17] or of hard-core bosons [18], being therefore integrable. The system remains integrable when the Ising interaction V_1 is added, no matter how large the anisotropy parameter μ is. The total Hamiltonian H_1 is known as the XXZ Hamiltonian and can be solved exactly via the Bethe ansatz [19].

In model 2, H_1 determines the mf basis and V_2 is treated as the "residual interaction" responsible for the onset of chaos. The parameter λ refers to the ratio between NNN and NN exchange.

Depending on the parameters of the Hamiltonians (1), different symmetries are identified [20]. For the sake of generality, we avoid them by restricting our analysis to a subspace with $L/3$ up spins and $\mu \neq 1$. We fix $\mu = 0.5$ for model 2. The only remaining symmetry is parity. We take it into account by studying only even states, which leads to subspaces of dimension $N \sim (1/2)L!/[(L/3)!(L - L/3)!]$. All data are given for $L = 15$.

Spectrum statistics.—According to the common lore, we analyze first the level spacing distribution $P(s)$ for both models, numerically obtained for different values of the control parameters μ and λ. For model 1, $P(s)$ is close to the Poisson distribution for any value of μ. For model 2, the transition of $P(s)$ from a Poisson to a Wigner-Dyson form as λ increases is shown in Fig. 1. The standard approach of fitting $P(s)$ with the Brody distribution [21] allows us to extract the repulsion parameter β characterizing the transition between the two distributions. From Fig. 1, the transition for model 2 occurs at $\lambda \approx 0.5$.

The transition of $P(s)$ from a Poisson to a Wigner-Dyson distribution is typical of nonintegrable systems of interacting particles. It was also seen in Bose-Hubbard models [22–24], which are of interest to experiments with optical lattices. The transition can occur both due to dynamical interaction only [22] and due to additional strong disorder [23]. The relevance of this transition to observable physical effects is discussed in Refs. [24].

Emergence of chaotic eigenstates.—Much more information about the systems is contained in the structure of the eigenstates. Our data show that as the strength of the perturbations V_1 and V_2 increases, the eigenstates of both

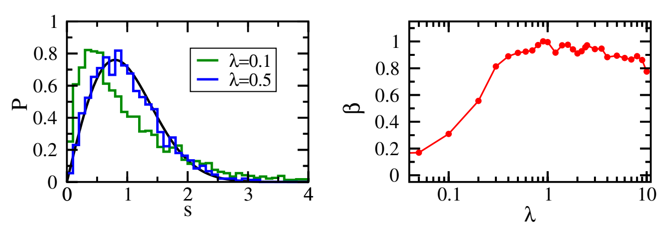

FIG. 1 (color online). Left: $P(s)$ for model 2 with $\lambda = 0.1, 0.5$ compared with the Wigner-Dyson distribution (smooth curve). Right: Brody parameter β as a function of λ.

integrable and nonintegrable models undergo a transition from localized to chaoticlike. Typical examples of the amplitudes C_n^α of such eigenstates with energy E_α from the center of the energy band are shown in Fig. 2. Here, the eigenstates are given as a function of the unperturbed energy ε_n rather than in the basis representation, following the one-to-one correspondence between $|n\rangle$ and its energy ε_n.

In order to find the critical parameters $\mu_{\rm cr}$ and $\lambda_{\rm cr}$ above which the perturbation is strong and the eigenstates are extended (in the energy shell), different approaches may be employed. We start by analyzing the matrix elements of H_1 and H_2. It is important to take into account that in each line n of the Hamiltonians, the perturbation couples directly only M_n unperturbed states [2,25]. We have numerically found that at the center of the energy band, $M_n \approx N/4$ and $M_n \approx N$ for models 1 and 2, respectively, (see [26] for more details). Thus, the Hamiltonian matrix of the integrable model is more sparse than the matrix of model 2.

To determine the critical perturbation, we compare the average value of the coupling strength, $v_n = \sum_{m\neq n}|H_{nm}|/M_n$, of each line n with the mean level spacing d_n between directly coupled states. The mean level spacing can be estimated as $d_n = [\varepsilon_n^{\rm max} - \varepsilon_n^{\rm min}]/M_n$, where $\varepsilon_n^{\rm max}$ ($\varepsilon_n^{\rm min}$) is the unperturbed energy corresponding to the largest (smallest) m where $H_{nm} \neq 0$. Our results show that for $\mu > \mu_{\rm cr} \approx 0.5$ and $\lambda > \lambda_{\rm cr} \approx 0.5$ the ratio v_n/d_n becomes larger than 1 and the perturbation is considered to be strong. Notice that for model 2, the obtained value of $\lambda_{\rm cr}$ corresponds to the onset of the Wigner-Dyson statistics, as independently found from the level spacing distribution. This is remarkable if we take into account that no diagonalization was necessary to derive the above estimates.

Strength function: From a Breit-Wigner to a Gaussian shape.—Another way to obtain the critical values $\mu_{\rm cr}$ and $\lambda_{\rm cr}$ relies on the shape of SF. The latter corresponds to the dependence of $w_n^\alpha = |C_n^\alpha|^2$ on the exact energies E_α for each fixed unperturbed energy ε_n. It contains information about the energies E_α that become accessible to an initial state $|n\rangle$ when the perturbation is turned on. Clearly, SF is related also to the structure of EFs, since the latter is derived from the same w_n^α, but now as a function of the unperturbed energies ε_n.

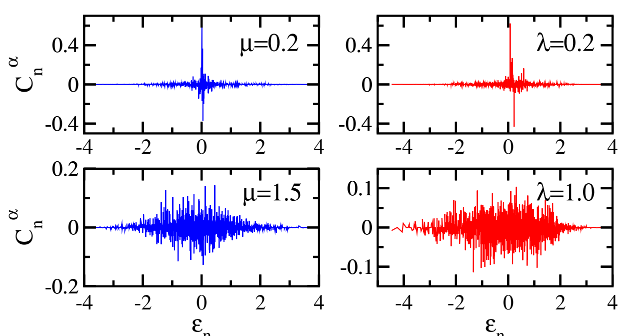

FIG. 2 (color online). Typical localized (top) and extended (bottom) eigenstates for model 1 (left) and model 2 (right).

In quantum many-body systems, the form of SF typically changes from Breit-Wigner to Gaussian as the interparticle interactions increase [2,6,8]. This transition occurs when the half-width of the Breit-Wigner distribution becomes comparable to the width of the energy shell. In this case, as we show next, there emerge chaotic eigenstates filling the whole available energy shell.

The energy shell corresponds to the distribution of states obtained from a matrix filled only with the off-diagonal elements of the perturbation. It is associated with the maximal SF, that is the SF that arises when the diagonal part of the Hamiltonian can be neglected. We verified that the energy shell coincides with a Gaussian of variance σ^2 given by the second moment of the off-diagonal elements of the matrix Hamiltonian, $\sigma^2 = \sum_{m\neq n}|H_{nm}|^2$ [2]. Note that no diagonalization is required to derive this expression.

Our numerical data confirm that the transition from a Breit-Wigner to a Gaussian shape occurs for the same critical values obtained above, $\mu_{\rm cr}$, $\lambda_{\rm cr} \approx 0.5$, as indicated in Fig. 3. In the figure, the envelopes of the SFs were obtained by smoothing the dependence of w_n^α on E_α for fixed unperturbed energies ε_n with $n \approx N/2$. The fit to either a Breit-Wigner or a Gaussian form was done with high accuracy, allowing us to discriminate between the two functions. It is noteworthy the excellent agreement between the Gaussian fit and the Gaussian obtained simply from the off-diagonal elements of the Hamiltonians.

Structure of eigenstates in the energy shell.—The eigenstates may be localized, sparse, or ergodically extended in the energy shell. The data in Fig. 4 demonstrate that for a

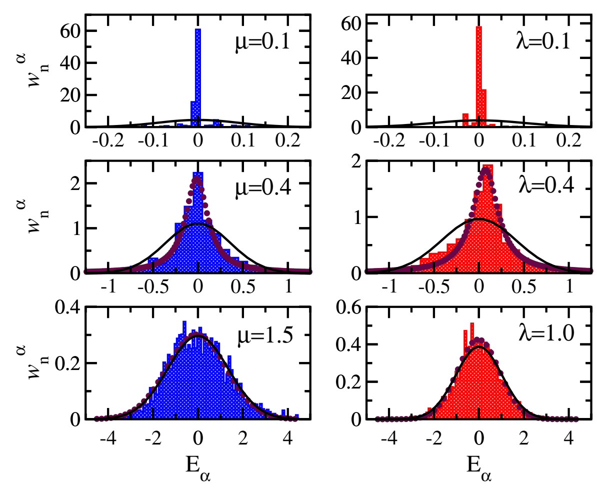

FIG. 3 (color online). Strength functions for model 1 (left) and model 2 (right) obtained by averaging over 5 close states in the middle of the spectrum. Middle panels: circles give a Breit-Wigner fit. Lower panels: circles stand for a Gaussian fit. In all panels, solid curves correspond to the Gaussian form of the energy shells.

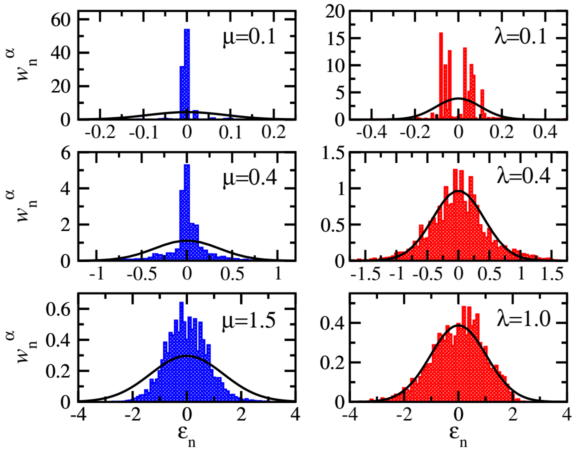

FIG. 4 (color online). Structure of eigenstates in the energy shells for model 1 (left) and model 2 (right) obtained by averaging over 5 states in the middle of the energy band. Solid curves correspond to the Gaussian form of the energy shell.

sufficiently strong perturbation the eigenstates undergo a transition from strongly localized to extended states, somehow filling the energy shell. The transition to chaoticlike eigenstates occurs again at the same critical parameters $\mu_{\rm cr}$, $\lambda_{\rm cr} \sim 0.5$. These results confirm the predictions made on the basis of both the estimate of v_n/d_n and the Gaussian form of the strength functions.

One notices that above the critical value, as shown by the bottom panels of Fig. 4, the eigenstates of model 1, differently from those of model 2, do not fill the entire energy shell, even for very strong perturbation. At the same token, a close inspection of the level of delocalization of individual EFs and SFs has revealed other differences between the two models. Overall, delocalization measures, such as the inverse participation ratio or the Shannon entropy, show larger fluctuations for model 1 than for model 2 [26]. This agrees with recent results obtained for bosonic and fermionic systems [15].

Statistical relaxation.—Reference [27] showed that when the two-body interaction between particles is completely random, allowing for an analysis in terms of two-body random ensembles, the quench dynamics can be described analytically. In our case, the two models are dynamical, without any randomness *ab initio*. Yet, we show below that when the interaction strength exceeds the critical value corresponding to the onset of chaoticlike eigenstates, the theory developed in Ref. [27] works perfectly for both integrable and nonintegrable models. This result is important in view of possible experimental observations in various systems of interacting spins-1/2.

By quench dynamics we mean the time evolution of initial states corresponding to unperturbed vectors which takes place once the interaction is turned on. To see how the relaxation occurs, we study the time dependence of the Shannon entropy S in the mf basis. For an initial state $|n_0\rangle$, it is defined as

$$S_{n_0}(t) = -\sum_{n=1}^{N} W_n(t)\ln W_n(t), \tag{2}$$

with $W_n(t) = |\sum_\alpha C_n^\alpha C_{n_0}^{\alpha*} e^{-iE_\alpha t}|^2$. To reduce fluctuations, we average over 5 initial basis states excited in a narrow energy range in the middle of the spectrum.

An analytical expression for $S_{n_0}(t)$ was derived in [27],

$$S_{n_0}(t) = -W_{n_0}(t)\ln W_{n_0}(t) - [1 - W_{n_0}(t)]\ln\left(\frac{1 - W_{n_0}(t)}{N_{\rm pc}}\right). \tag{3}$$

Here $W_{n_0}(t)$ is the probability for the system to stay in the initial state $|n_0\rangle$ and $N_{\rm pc}$ is the average number of directly coupled states. We obtain $N_{\rm pc}$ numerically according to $N_{\rm pc} = \langle e^S\rangle$, where the average $\langle . \rangle$ is performed over a long time after the saturation of the entropy.

Figure 5 shows numerical data for the relaxation process of both models. Initially, the entropy grows quadratically, as given by perturbation theory. Afterwards, a clear linear growth is observed before $S(t)$ reaches relaxation. With high accuracy the linear behavior of $S(t)$ is described by the simple relation [27],

$$S_{n_0}(t) \approx \sigma_{n_0} t \ln M_{n_0}. \tag{4}$$

Note that Eq. (4) depends only on the elements of the Hamiltonian: $\sigma_{n_0}^2 = \sum_{m\neq n_0}|H_{n_0 m}|^2$ and M_{n_0} is the connectivity of line n_0. As seen in Fig. 5, the analytical expressions (3) and (4) give a correct description of the entropy growth for both models in the regime corresponding to the onset of chaoticlike eigenstates delocalized in the energy shell. The same relation (4) was found to emerge also for an integrable model of interacting bosons [28].

Conclusion.—We have studied the spectrum statistics, the structures of eigenstates and strength functions, and the quench dynamics for two models of interacting spins, connecting the results with the onset of chaotic eigenstates and the emergence of statistical relaxation. The key point of our approach is the existence of an energy shell of finite range, inside which the eigenfunctions can be either localized or extended. We have shown that the critical parameters above which the eigenstates become chaoticlike can be

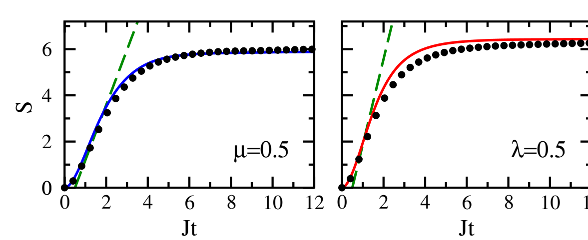

FIG. 5 (color online). Shannon entropy vs rescaled time for model 1 (left) and model 2 (right) for strong perturbation. Circles stand for numerical data, solid curves correspond to Eq. (3), and dashed lines show the linear dependence (4).

equally found by simply studying the elements of the Hamiltonian or by analyzing the shape of the strength function. The latter provides the form of the energy shell, thus allowing one to clearly define the notion of delocalized eigenstates in the energy shell.

Our study shows that Wigner-Dyson level statistics is not important for the onset of statistical relaxation. Indeed, by studying the time dependence of the Shannon entropy, we have shown that numerical data are in full agreement with the analytical predictions of the quench dynamics, provided the eigenstates are chaoticlike. In this case, the relaxation process for both integrable and nonintegrable systems becomes very similar. This result does not contradict the eigenstate thermalization hypothesis, but identifies the primary conditions for the thermalization of isolated quantum systems. Our approach is very general and expected to apply to different systems of interacting particles, such as those currently under theoretical and experimental investigation.

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