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Memory of the Initial Conditions in an Incompletely-Chaotic Quantum System: Universal Predictions and an Application to Cold Atoms

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Two zero-range-interacting atoms in a circular, transversely harmonic waveguide are used as a test-bench for a quantitative description of the crossover between integrability and chaos in a quantum system with no selection rules. For such systems we show that the expectation value after relaxation of a generic observable is given by a linear interpolation between its initial and thermal expectation values. The variable of this interpolation is universal; it governs this simple law to cover the whole spectrum of the chaotic behavior from integrable regime through the well-developed quantum chaos. The predictions are confirmed for the waveguide system, where the mode occupations and the trapping energy were used as the observables of interest; a variety of the initial states and a full range of the interaction strengths have been tested.

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Two distinct types of evolution of an isolated dynamical system are usually identified: a predictable evolution, strongly correlated with the initial state on one hand and a relaxation to the thermal equilibrium with no memory of the initial state on the other. An ideal gas of non-interacting atoms is a trivial example of a predictable evolution. In cold quantum gases, this type of behavior was observed for the single-mode excitations in Bose-Einstein condensates [1, 2] and a one-dimensional gas of interacting atoms [3]. Such systems can be described by integrable models, i.e. models that have as many integrals of motion as there are degrees of freedom. Lifting of integrability leads to a chaotic motion. For ultracold atoms, notable examples of the quantum-chaotic motion include both a non-stationary δ-kicked rotor [4, 5] and a stationary billiard [6].

Interactions between the trapped atoms are the most common cause of integrability lifting (with the exception of the one-dimensional gas, see [7]). Even for the case of just two trapped atoms, interactions can already destroy integrability [8]. For ultracold atoms, the atomic de Brogle wavelength typically substantially exceeds the interaction range. In this case, the interaction couples every two eigenstates of non-interacting atoms with approximately the same strength, yielding no selection rules interaction can obey.

In this Letter, we analyze the case of two interacting atoms in a circular, transversely harmonic waveguide in the multimode regime [8]. Similar models, the Šeba billiard [9] and a cylindrically-symmetric harmonic trap with a δ-scatterer [10], were considered by other authors as well. These models, as well as the waveguide model, are non-integrable and show some signatures of a quantum-chaotic behavior as a result. However, their behavior is only incompletely-chaotic, since the systems demonstrate some substantial deviations from quantum-chaotic predictions as well (see [8, 11] and the references therein). In these systems, the interaction strength can be used to tune the "chaoticity".

Trajectories of a completely-chaotic classical system fill all the available phase space in a "mixing" motion. This leads to a relaxation to the thermal equilibrium. In quantum systems relaxation to the thermal equilibrium—predicted by the Gibbs ensemble—is ensured by the effect of eigenstate thermalization [12–14]. The relaxation property can be considered as one of the criteria of chaotic behavior. Evolution of an integrable system preserves the integrals of motion and its state after relaxation is characterized by the generalized Gibbs ensemble [15]. It should be noted that completely-chaotic systems are as rare as integrable systems.

In classical systems, the KAM theory predicts a continuous crossover between the regular and chaotic regimes, controlled by the system parameters. For quantum systems, a smooth breakdown of thermalization was demonstrated for hard-core bosons on a finite lattice [16]. In this Letter, we offer an approximate analytic prediction for the state after relaxation of general quantum systems with no selection rules (e.g., models [8–10] and an embedded random matrix model [17]). The resulting expression smoothly covers the space between the integrable and quantum-chaotic regimes as a function of an universal parameter which is the same for all observables and insensitive to the initial state. Unlike the predictions for completely-chaotic [14] and integrable [15] systems, the equilibrium-state universality is not governed by the conserved quantities alone but rather by some universal traits in how the integrals of motion can be broken. The prediction is tested against the exact analytic results for the waveguide system. This system seems to be ex-

perimentally realizable, as individually-trapped pairs of ultracold atoms are already used in recent experiments (see [18] and references therein).

Consider an integrable (IS) and a non-integrable (NS) systems with Hamiltonians $\hat{H}_0$ and $\hat{H} = \hat{H}_0 + \hat{V}$, eigenstates $|\vec{n}\rangle$ ($\vec{n}$ is an appropriate set of quantum numbers) and $|\alpha\rangle$ (energy ordered), and eigenenergies $E_{\vec{n}}$ and E_α, respectively. The Schrödinger equation for NS readily gives

$$|\alpha\rangle = \sum_{\vec{n}} \frac{|\vec{n}\rangle\langle\vec{n}|\hat{V}|\alpha\rangle}{E_\alpha - E_{\vec{n}}}. \tag{1}$$

Given a non-equilibrium initial state $\hat{\rho}_{\rm in} \equiv \hat{\rho}(t=0)$, where $\hat{\rho}(t)$ is the NS density matrix, the expectation value of a generic observable $\hat{A}$ of NS relaxes to the infinite time average (see [14])

$$A_{\rm rel} \equiv \lim_{T\to\infty} \frac{1}{T}\int_0^T dt {\rm Tr}\left(\hat{A}\hat{\rho}(t)\right) = \sum_\alpha \langle\alpha|\hat{\rho}_{\rm in}|\alpha\rangle\langle\alpha|\hat{A}|\alpha\rangle. \tag{2}$$

First, consider the case when (a) initial density matrix is diagonal in the IS basis, $\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle = \rho^{\rm in}_{\vec{n}}\delta_{\vec{n}\vec{n}'}$, and (b) the observable is an integral of motion of the IS, $\langle\vec{n}|\hat{A}|\vec{n}'\rangle = A_{\vec{n}}\delta_{\vec{n}\vec{n}'}$. Using the partial fraction decomposition, Eqs. (1) and (2) can be transformed, with no approximations, to

$$A_{\rm rel} = \sum_{\vec{n}} A_{\vec{n}}\eta_4(E_{\vec{n}})\rho^{\rm in}_{\vec{n}} + \sum_{\vec{n}\neq\vec{n}'} A_{\vec{n}}F_{\vec{n}\vec{n}'}\rho^{\rm in}_{\vec{n}'}, \tag{3a}$$

$$F_{\vec{n}\vec{n}'} = \frac{\eta^{(2)}_{\vec{n}\vec{n}'\vec{n}\vec{n}'}(E_{\vec{n}}) + \eta^{(2)}_{\vec{n}\vec{n}'\vec{n}\vec{n}'}(E_{\vec{n}'})}{(E_{\vec{n}} - E_{\vec{n}'})^2} + 2\frac{\eta^{(1)}_{\vec{n}\vec{n}'\vec{n}\vec{n}'}(E_{\vec{n}}) - \eta^{(1)}_{\vec{n}\vec{n}'\vec{n}\vec{n}'}(E_{\vec{n}'})}{(E_{\vec{n}'} - E_{\vec{n}})^3} \tag{3b}$$

$$\eta^{(j)}_{\vec{n}\vec{n}'\vec{n}''\vec{n}'''}(E) = \sum_\alpha \frac{V_{\vec{n}\alpha}V_{\vec{n}'\alpha}V_{\alpha\vec{n}''}V_{\alpha\vec{n}'''}}{(E_\alpha - E)^j}. \tag{3c}$$

Here

$$\eta_4(E_{\vec{n}}) = \eta^{(4)}_{\vec{n}\vec{n}\vec{n}\vec{n}}(E_{\vec{n}}) \equiv \sum_\alpha |\langle\vec{n}|\alpha\rangle|^4 \tag{4}$$

is the inverse participation ratio (IPR) [19]. Its inverse estimates the number of the NS eigenstates the IS one consists of. IPR can be considered as a measure of "chaoticity" of the system, since it varies from 1 for IS to $\eta_4(E_{\vec{n}}) \ll 1$ for a completely-chaotic system.

Diagonal matrix elements $A_{\vec{n}}$ of a typical observable $\hat{A}$ can be decomposed into a sum of a smooth function of the state energy $E_{\vec{n}}$ and fluctuations around it. One can introduce a macroscopic energy scale $\Delta_{\rm MS}$—an energy over which the smooth part does not change substantially. Now, assume that the function $F_{\vec{n}\vec{n}'}$ decays at the energy distances $|E_{\vec{n}} - E_{\vec{n}'}|$ less than $\Delta_{\rm MS}$. Let us also introduce a set of intervals $[\mathcal{E}_i, \mathcal{E}_{i+1}]$ and the function $B_i(\vec{n}) = \sum_{\vec{n}',\vec{n}'\neq\vec{n},\mathcal{E}_i<E_{\vec{n}'}<\mathcal{E}_{i+1}} F_{\vec{n}\vec{n}'}\rho^{\rm in}_{\vec{n}'}$, which is localized in some energy window $E_{\vec{n}} \in \mathcal{W}_i$. For a sufficiently small interval $[\mathcal{E}_i, \mathcal{E}_{i+1}]$ the energy window $\mathcal{W}_i$ will become smaller than or comparable to $\Delta_{\rm MS}$.

We consider here a system with no selection rules, i.e. we assume that $V_{\vec{n}\vec{n}'}$ do not show any systematic dependence on the differences between the quantum numbers $\vec{n}$ and $\vec{n}'$. Two distinct classes of such interactions are the zero-range interactions considered below and the random-matrix interactions (see [17]). In the absence of the selection rules, the only systematic dependence between eigenstates $\vec{n}$ and $\vec{n}'$, coupled by the function $F_{\vec{n}\vec{n}'}$ can be due to the energy denominators in Eq. (3b) selecting energy-neighboring states. However, in the generic case, different degrees of freedom of the IS have incommensurate frequencies. As a result, the quantum numbers of highly-excited energy-neighboring states will be mutually uncorrelated and $B_i(\vec{n})$ is indiscriminate with respect to the quantum number values available in the window $\mathcal{W}_i$, even if IS eigenstates $\vec{n}'$ in the initial state are specially selected according to their quantum numbers. Consequently, the sequences $A_{\vec{n}}$ and $B_i(\vec{n})$ become uncorrelated. Mathematically this means that their correlation function is equal to the product of their mean values, $\sum_{\vec{n}} A_{\vec{n}}B_i(\vec{n})/\mathcal{N}_i \approx A_{\rm MC}((\mathcal{E}_i + \mathcal{E}_{i+1})/2)\sum_{\vec{n}} B_i(\vec{n})/\mathcal{N}_i$. Provided a statistically sufficient number of IS eigenstates $\mathcal{N}_i$ in the window $\mathcal{W}_i$,

$$A_{\rm MC}((\mathcal{E}_i + \mathcal{E}_{i+1})/2) = \frac{1}{\mathcal{N}_i}\sum_{\vec{n},E_{\vec{n}}\in\mathcal{W}_i} A_{\vec{n}} \tag{5}$$

expresses the definition of the microcanonical expectation value. Equation (3a) is reduced then to

$$A_{\rm rel} \approx \sum_{\vec{n}} \left[A_{\vec{n}}\eta_4(E_{\vec{n}}) + A_{\rm MC}(E_{\vec{n}})(1 - \eta_4(E_{\vec{n}}))\right]\rho^{\rm in}_{\vec{n}}. \tag{6}$$

[Here orthogonality and completeness of the basis set $|\alpha\rangle$ are used and $A_{\rm MC}((\mathcal{E}_i + \mathcal{E}_{i+1})/2)$ is approximated by $A_{\rm MC}(E_{\vec{n}})$.] Further, we can approximate IPR by its average value over the initial state $\bar{\eta} = \sum_{\vec{n}} \eta_4(E_{\vec{n}})\rho^{\rm in}_{\vec{n}}$, getting

$$A_{\rm rel} \approx \bar{\eta}A_{\rm in} + (1 - \bar{\eta})A_{\rm therm} \tag{7}$$

$$A_{\rm in} = \sum_{\vec{n}} A_{\vec{n}}\rho^{\rm in}_{\vec{n}}, \quad A_{\rm therm} = \sum_{\vec{n}} A_{\rm MC}(E_{\vec{n}})\rho^{\rm in}_{\vec{n}}. \tag{8}$$

This expression has a clear physical meaning. An initial state populates $\sim \bar{\eta}^{-1}$ states of NS per each IS state $|\vec{n}\rangle$ contained in the initial state. Since weight of each of the NS state in $|\vec{n}\rangle$ is $\sim \bar{\eta}$ and vice versa, the contribution of $|\vec{n}\rangle$ into the equilibrium state will be proportional to $\bar{\eta}$. Other IS states, contained in the populated NS states, give a thermal contribution of a weight $1 - \bar{\eta}$. In the case of IS, $\bar{\eta} = 1$ and the system keeps initial expectation value of the observable $A_{\rm in}$; on the other hand,

for completely-chaotic systems, where $\bar{\eta} \ll 1$, it relaxes to the microcanonical expectation value, averaged over the initial state, i.e. to $A_{\rm therm}$. If $\Delta_{\rm MS}$ is greater then the energy width of the initial state with the energy E, $A_{\rm therm} \approx A_{\rm MC}(E)$ and the memory of initial conditions is given by the first term in Eq. (7) only. However, for broad initial states, $A_{\rm therm}$ depends on $\hat{\rho}_{\rm in}$ as well; in this case, some memory of initial conditions will be retained, even in the completely-chaotic regime.

Since averages over intervals $[\mathcal{E}_i, \mathcal{E}_{i+1}]$ fluctuate independently, the accuracy of Eq. (6) is determined by the total number of IS eigenstates $\mathcal{N}_{\rm A}$ which are effectively involved in the summation over $\vec{n}$ in the second term of Eq. (3a). Since each eigenstate $\vec{n}'$ in the initial state provides $\sim \bar{\eta}^{-1}(1-\bar{\eta}^{-1})$ eigenstates $\vec{n}$ to the state after relaxation,

$$\mathcal{N}_{\rm A} \sim \frac{\mathcal{N}_i A_{\rm MC}(E)^2}{\sum_{\vec{n}, E_{\vec{n}} \in \mathcal{W}_i} A_{\vec{n}}^2} \bar{\eta}^{-1}(1-\bar{\eta}^{-1}) \left[\sum_{\vec{n}'} \left(\rho_{\vec{n}'}^{\rm in}\right)^2 \right]^{-1} . \quad (9)$$

Here the last factor gives number of eigenstates in the initial state and the first one estimates part of eigenstates selected by the observable $\hat{A}$ (it is approximately independent of the interval $\mathcal{W}_i$ containing E). The applicability criterion would be $\mathcal{N}_{\rm A} \gg 1$.

Below, we verify the prediction (7) and (8) using an example of two ultracold trapped atoms [8]. The interaction is approximated by the zero-range Fermi-Huang pseudopotential $\hat{V} = (2\pi\hbar^2 a_s/\mu)\delta_3(\boldsymbol{r})(\partial/\partial r)(r\,\cdot)$ (its applicability to ultracold collisions was widely confirmed, see e.g. [20]). Here a_s is the three-dimensional s-wave scattering length, μ is the reduced mass of the colliding atoms, and $\boldsymbol{r}$ is the relative coordinate. The atoms are trapped in a cylindrical harmonic potential with the frequency $\omega_\perp$. The ring geometry of the waveguide imposes period-L boundary conditions along the potential axis. This model allows separation of the center-of-mass motion, leaving a system with two degrees of freedom, the axial z and radial ρ relative coordinates. The eigenstates of non-interacting IS $|nl\rangle$ are products of the axially-symmetric wavefunction $|n\rangle$ of two-dimensional harmonic oscillator and a symmetric plane wave with the momentum $2\pi l\hbar/L$ (states of other symmetry are not coupled by the zero-range interaction). For the zero-range potential, Eq. (1) expresses the eigenstate $|\alpha\rangle$ in an explicit form [8–10], which involves only a few states $|\vec{n}\rangle$ with closest energy. Such systems do not approach the regime of a complete chaos, even for strong interaction; accordingly, their IPR remains relatively large in this regime. The present waveguide system retains $\bar{\eta} \gtrsim 0.39$ even when it approaches the maximally-chaotic regime (see [8]) at $a_s > 0.1 a_\perp$, where $a_\perp = (\hbar/\mu\omega_\perp)^{1/2}$ is the transverse oscillator range. The aspect ratio is chosen as a large transcendental number $L/a_\perp = \pi^{7/2}(1+\sqrt{5})^{1/2} \approx 99$, where the system behavior appears to be more chaotic.

Having in mind the further comparison with the case

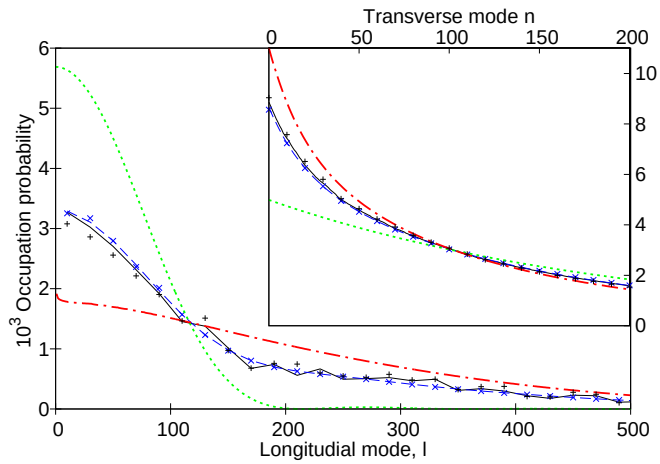

FIG. 1: (Color online) Distributions over the transverse (insert) and longitudinal modes of the integrable system. The infinite-time average (2) [black solid line] is compared to predictions (6) with state-dependent IPR [crosses] and (7) with averaged IPR $\bar{\eta} = 0.39$ (blue dashed line) in the strong-interaction regime $a_s = 10^6 a_\perp$ for the initial state (10) with $\kappa = 400$ and $\delta \approx 7\times10^{-3}$. The dotted (green) and dot-dashed (red) lines show the initial distributions and the averaged microcanonical predictions (8). The infinite-time average for the non-diagonal initial density matrix is shown with pluses.

of non-diagonal initial state, we consider the diagonal matrix $\rho_{nl}^{\rm in} = |\langle\psi_{\rm in}|nl\rangle|^2$ with

$$\langle z, \rho|\psi_{\rm in}\rangle \propto \cos\frac{\pi\zeta}{\delta}\theta\left(\frac{\delta}{2} - |\zeta|\right)\exp\left(-\frac{\kappa\rho^2}{a_\perp^2}\right) \quad (10)$$

and $\zeta = z/L - 1/2$ (see [8]).

Figure 1 demonstrates a good agreement between the predictions (6) and the infinite time average (2) for distributions over transverse and longitudinal modes described by operators $|n\rangle\langle n|$ and $\frac{1}{20}\sum_{l'=l-9}^{l+10}|l'\rangle\langle l'|$, respectively. It also shows that predictions for constant IPR (7) and state-dependent IPR (6) almost coincide.

Consider now the more general case when the initial density matrix has non-diagonal elements in the IS basis. Infinite-time average can be expressed like Eq. (3a). The contributions of alternating-sign sums $\eta^{(j)}_{\vec{n}\vec{n}'\vec{n}''\vec{n}'''}(E)$ with odd j can be neglected. Neglecting also alternating-sign terms with the odd powers of energy differences of the involved IS states, we obtain the correction to Eq. (3a)

$$A_{{\rm nd}\rho} = -2{\rm Re}\sum_{\vec{n}\neq\vec{n}'} A_{\vec{n}}\eta^{(2)}_{\vec{n}'\vec{n}\vec{n}\vec{n}}(E_{\vec{n}})\frac{\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle}{(E_{\vec{n}} - E_{\vec{n}'})^2} \quad (11)$$

This correction is small if the non-diagonal matrix elements of $\hat{\rho}_{\rm in}$ have arbitrary phase or if the non-equilibrium initial state does not contain energy-neighboring modes $\vec{n}$ and $\vec{n}'$ (note, that uniform occupation of all modes corresponds to the thermal equilibrium). The initial state of the form $\langle nl|\hat{\rho}_{\rm in}|n'l'\rangle =$

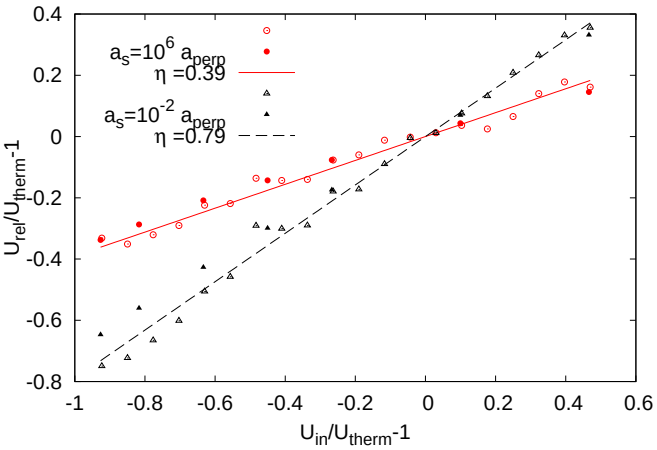

FIG. 2: (Color online) The solid (red) and dashed (black) lines show predictions (7) for expectation values of the transverse potential energy U for strong ($a_s = 10^6 a_\perp$, $\bar{\eta} = 0.39$) and weak ($a_s = 10^{-2} a_\perp$, $\bar{\eta} = 0.79$) interactions, respectively, in comparison to the infinite-time average (circles and triangles, respectively). The filled and open symbols correspond to initial states (10) and (13), respectively. For all the points the system energy is $E \approx 205\hbar\omega_\perp$.

$\langle nl|\psi_{\rm in}\rangle\langle\psi_{\rm in}|n'l'\rangle$, used in Fig. 1, could lead to large corrections since the non-diagonal terms are comparable to the diagonal ones and for the state (10) overlaps $\langle nl|\psi_{\rm in}\rangle$ have positive and substantial values for $\sim \kappa$ transverse and $\sim \delta^{-1}$ longitudinal successive modes. Nevertheless, even in this case results for diagonal and non-diagonal initial states are pretty close (for other parameters ranges and initial states the discrepancy is even smaller).

Consider now the most general case when both $\hat{\rho}_{\rm in}$ and the observable $\hat{A}$ have non-diagonal elements in the IS basis. In this case, the value $A_{\rm in}$ defined by Eq. (8) is different from the actual initial expectation value. Rather, it corresponds to the infinite-time average for evolution of IS. In addition, the correction to Eq. (3a)

$$A_{{\rm nd}A} = -4{\rm Re}\sum_{\vec{n}\neq\vec{n}'}\frac{\langle\vec{n}|\hat{A}|\vec{n}'\rangle}{(E_{\vec{n}}-E_{\vec{n}'})^2}\left[\eta^{(2)}_{\vec{n}'\vec{n}\vec{n}\vec{n}}(E_{\vec{n}})\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}\rangle\right.$$
$$\left.-\eta^{(2)}_{\vec{n}\vec{n}'\vec{n}\vec{n}'}(E_{\vec{n}})\langle\vec{n}'|\hat{\rho}_{\rm in}|\vec{n}\rangle-\eta^{(2)}_{\vec{n}'\vec{n}'\vec{n}\vec{n}}(E_{\vec{n}})\langle\vec{n}|\hat{\rho}_{\rm in}|\vec{n}'\rangle\right] \quad (12)$$

can be derived in the same way as Eq. (11). This correction is small if the operator $\hat{A}$ does not couple energy-neighboring states of the integrable system (it is a characteristic property of observables which do not act on some degrees of freedom).

As a concrete example of an observable we take the transverse potential energy $\hat{U} = \mu\omega_\perp^2\rho^2/2$. This observable couples the states with $l' = l$ and $n' = n, n\pm 1$. Therefore $|E_{\vec{n}} - E_{\vec{n}'}| = 2\hbar\omega_\perp$ and the denominator in Eq. (12) is large. Figure 2 demonstrates good agreement between Eq. (7) and exact results. Both the initial state (10) and the initial state

$$\langle z,\rho|\psi_{\rm in}\rangle \propto \cos\frac{\pi\zeta}{\delta}\theta\left(\frac{\delta}{2}-|\zeta|\right)\cos\left(2\pi l_0\zeta\right)|n_0\rangle \quad (13)$$

were used. This state consists of two wavepackets moving in mutually opposite directions along the waveguide axis (reminiscent of the experiment [3]). Two completely different interaction strengths determine, with a good accuracy, the IPR values, which, for a given energy, are insensitive to the nature of the initial state .

In conclusion, we demonstrate that an incompletely-chaotic non-integrable systems with no selection rules relaxes to an equilibrium state which keeps a predictable memory of the initial state. We show that the value after relaxation of a generic observable is given by a linear interpolation (7) between the thermal expectation value and the prediction of the "diagonal ensemble" for the underlying integrable system (8). The variable of this interpolation—the IPR (4)—is universal: it is the same for all system observables and insensitive to the shape of the initial state. Microcanonical prediction further averaged over the initial state should be used as the thermal expectation value (8). This prediction is in a good agreement with the exact results on the relaxation in a system of two zero-range-interacting atoms in a circular, transversely harmonic waveguide.

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