Nonlinear Perturbation of Random Matrix Theory

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We consider a system of linear oscillators, or quantum states, described by random matrix theory and analyze how its time evolution is affected by a nonlinear perturbation. Our numerical results show that above a certain chaos border a weak or moderate nonlinearity leads to a dynamical thermalization of a finite number of degrees of freedom with energy equipartition over linear eigenmodes as expected from the laws of classical statistical mechanics. The system temperature is shown to change in a broad range from positive to negative values, and the dependence of system characteristics on the initial injected energy is determined. Below the chaos border the dynamics is described by the Kolmogorov-Arnold-Moser integrability. Owing to universal features of random matrix theory we argue that the obtained results describe the generic properties of its nonlinear perturbation.

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In far 1872, 150 years ago, Boltzmann developed the theory of statistical mechanics and thermalization originated from the dynamical laws of classical motion of many-body systems [1]. This result led to the famous Boltzmann-Loschmidt dispute on a possibility of thermalization and time irreversibility emerging from the reversible dynamical equations of particle motion [2,3] (see also Ref. [4]). The modern resolution of this dispute is based on the theory of dynamical chaos for generic nonlinear systems characterized by a positive maximal Lyapunov exponent and Kolmogorov-Sinai entropy leading to an exponential instability of motion (see, e.g., Refs. [5–8]). This instability leads to an exponential growth of errors which breaks time reversibility (see, e.g., an example in Ref. [9]).

The first numerical studies of how ergodicity, dynamical thermalization, and energy equipartition appear in a homogeneous 1D oscillator chain perturbed by a moderate nonlinearity were reported by Fermi, Pasta, Ulam in 1955 [10] (see system Hamiltonian in the Supplemental Material [11]). The conclusion was that "The results show very little, if any, tendency toward equipartition of energy between the degrees of freedom" [10]. It was argued in Ref. [18] that in the continuum limit the Fermi-Pasta-Ulam (FPU) problem is close to the Korteweg-de Vries equation with stable soliton solutions shown to be completely integrable [19], as well as the nonlinear Schrödinger equation [20]. In addition, at weak nonlinearity the FPU α model is close to the completely integrable Toda lattice [21,22]. Another explanation of equipartition absence in the FPU problem was given in Refs. [23–25] showing that below a certain strength of nonlinear interactions between oscillator modes the system is located in the regime of Kolmogorov-Arnold-Moser (KAM) integrability, and only above this border an overlap of nonlinear resonances takes place with the emergence of chaos and thermalization. Numerical simulations demonstrated a dynamical thermalization with energy equipartition reported in Refs. [24,25]. Thus, even 50 years after [10], various regimes of nonlinear dynamics of the FPU problem are actively discussed by the community of dynamical systems [26] (see, e.g., recent Ref. [27]). The variety of studies clearly demonstrates that this model played an important role in the investigations of nonlinear dynamics but also that it has multiple specific features indicating that it does not belong to a class of generic oscillator systems with nonlinear interactions.

To construct a generic model of many-body oscillator systems with nonlinear interactions between oscillators we take insight from quantum mechanics of many-body systems whose spectral properties are described by random matrix theory (RMT) invented by Wigner for a description of the spectra of complex nuclei, atoms, and molecules [28]. At present RMT finds applications in multiple areas of physics [29,30] including systems of quantum chaos whose dynamics is chaotic in the classical limit [31,32]. The properties of RMT eigenvalues and eigenstates were established in various studies and are well known. The RMT eigenstates are ergodic, i.e., uniformly distributed on the N-dimensional unit sphere, and the level spacing statistics is described by the universal RMT distribution [28–32]. Owing to the linearity of the Schrödinger equation the time evolution of a wave function ψ described by a RMT Hamiltonian also describes a time evolution of a system of N linear oscillators with random linear couplings. On its own, because of the universal properties of RMT, it is interesting to understand how a nonlinear perturbation affects RMT evolution.

With the aim of understanding the effects of nonlinear perturbation of RMT, we consider a simple model

described by the Schrödinger equation with a Hamiltonian given by a random matrix with an additional nonlinear interaction between linear modes:

$$i\hbar\frac{\partial\psi_n(t)}{\partial t}=\sum_{n'=1}^{N}H_{n,n'}\psi_{n'}(t)+\beta|\psi_n(t)|^2\psi_n(t). \quad (1)$$

Here $H_{n,n'}$ are elements of an RMT matrix $\hat{H}$ of size N taken from the Gaussian orthogonal ensemble (GOE) [29]; they have zero mean and variance $\langle H_{n,n'}^2\rangle=(1+\delta_{n,n'})/[4(N+1)]$. The averaged density of states is given by the semicircle law $dm/dE=(2N/\pi)\sqrt{1-E^2}$ with typical eigenvalues in the interval $E_m\in[-1,1]$ (we use dimensionless units with $\hbar=1$), and β is a dimensionless constant characterizing the nonlinear interaction strength in the original basis n.

The eigenmodes of $\hat{H}$ at energies E_m are $\phi_n^{(m)}$ which are ergodic with a uniform distribution on the N-dimensional unit sphere. The time evolution of the wave function can be expressed in the basis of eigenmodes as $\psi_n(t)=\sum_{m=1}^{N}C_m(t)\phi_n^{(m)}$ with coefficients $C_m(t)$ giving the occupation probability $\rho_m=\langle|C_m(t)|^2\rangle$ (with some long time or ensemble average; see below). The time evolution [Eq. (1)] has two integrals of motion being the probability norm $\sum_n|\psi_n(t)|^2=1$ and total energy $E=\sum_n[\langle\psi_n(t)|\hat{H}|\psi_n(t)\rangle+(\beta/2)|\psi_n(t)|^4]$. At $\beta=0$ the model [Eq. (1)] can be viewed as a quantum system or as a classical system of coupled linear oscillators whose Hamiltonian in the basis of oscillator eigenmodes is $\mathcal{H}=\sum E_mC_m^*(t)C_m(t)$ where C_m, C_m^* is a pair of conjugated variables and E_m plays the role of oscillator frequencies. Since RMT captures the universal features of quantum and linear oscillator systems we expect that the model [Eq. (1)] describes the universal properties of oscillator systems with chaotic dynamics induced by weak or moderate nonlinear couplings between oscillators. We call the model [Eq. (1)] the nonlinear random matrix model (NLIRM).

Above a certain chaos border with $\beta>\beta_c$ a moderate nonlinearity destroys KAM integrability leading to chaotic dynamics with a positive maximal Lyapunov exponent λ. The nonlinear frequency shift is $\delta\omega\sim\beta|\psi_n|^2\sim\beta/N$ and, as it was argued in Refs. [33–36], a developed chaos takes place when this shift $\delta\omega$ becomes comparable to a typical energy spacing between energies (or frequencies) of the linear system $\Delta\omega\sim 1/N$. Thus $\delta\omega>\Delta\omega$ implies chaos with the chaos border $\beta_c=\text{const}\sim 1$ being independent of system size N.

The issue of dynamical thermalization in finite size nonlinear lattices with disorder was studied in Refs. [36,37]. The time evolution in these systems is described by the discrete Anderson nonlinear Schrödinger equation (DANSE) with hopping between nearby sites (see DANSE in the Supplemental Material [11]). In the linear case the disorder leads to Anderson localization of modes [38] which is well visible when the localization length ℓ is smaller than the system size N. In this respect our RMT model [Eq. (1)] is rather different since the linear modes are delocalized and ergodic in a vector space of dimension N. We expect that our model [Eq. (1)] is generic and captures also certain features of the models of the Bose-Einstein condensate evolution in the chaotic Bunimovich stadium [39] or the Sinai oscillator [40] described by the nonlinear Gross-Pitaevskii equation (GPE) [41] (see GPE in the Supplemental Material [11]). Indeed, the linear eigenmodes of these systems have properties of quantum chaos similar to RMT [31,32]. There are however also certain differences discussed below.

For the GPE models [39,40] it is natural to assume that the dynamical thermalization induced by moderate nonlinearity leads to the Bose-Einstein (BE) distribution of probabilities ρ_m over quantum levels of the linear system. In the limit of high temperature T this distribution is reduced to a classical energy equipartition (EQ) distribution [4,42]. For the DANSE type models [36,37] the quantum Gibbs (QG) distribution was proposed to explain numerically obtained results. In fact QG and BE distributions give very close thermalization properties, and we mainly discuss the BE case here. Thus there are two options for the thermalized distributions of probabilities ρ_m:

$$\rho_m=\frac{1}{\exp[(E_m-\mu)/T]-1}\,(\text{BE}),\qquad \rho_m=\frac{T}{E_m-\mu}\,(\text{EQ}). \quad (2)$$

Here T is the system temperature and $\mu(T)$ is the chemical potential dependent on temperature. The parameters T and μ are determined by the norm and energy conservation $\sum_m\rho_m=1$ and $\sum_m E_m\rho_m=E$ (for E we assume the case of weak or moderate nonlinearity which gives only a weak contribution to the total energy). The entropy S of the system is determined by the usual relation [4,42]: $S=-\sum_m\rho_m\ln\rho_m$ with the implicit theoretical dependencies on temperature $E(T), S(T), \mu(T)$. The derivation of Eq. (2) is given in the Supplemental Material [11].

Based on classical statistical mechanics [4,42] the dynamical thermalization should lead to the EQ distribution [Eq. (2)] since the DANSE, GPE [36,37,39,40], and NLIRM [Eq. (1)] models describe classical nonlinear fields without second quantization. In contrast, in Refs. [36,37,39,40] it was argued that a moderate nonlinearity plays the role of an effective nonlinear thermostate that leads to quantum BE or QG distributions [Eq. (2)].

Of course, both BE and EQ approaches [Eq. (2)] give different thermal characteristics leading to a contradiction discussed in detail in Refs. [37,39,40]. The main argument in favor of the BE (or the QG) ansatz was based on a reasonably good agreement of numerical data for entropy vs energy with the theoretical thermal dependence $S(E)$

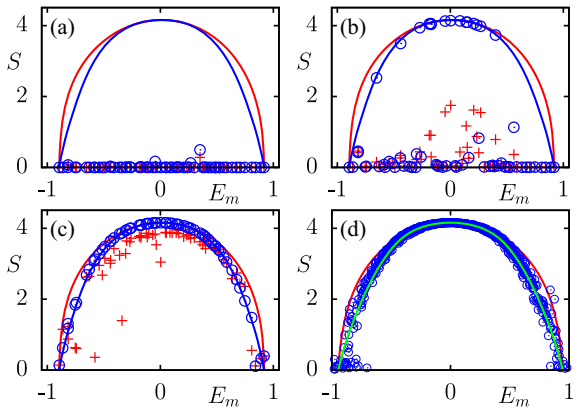

FIG. 1. Entropy S versus energy E_m of the initial state m at $t = 0$ for one RMT realization at $N = 64$ and $\beta = 0.02$ (a), $\beta = 0.1$ (b), and $\beta = 1$ (c) or 10 RMT realizations at $\beta = 1$ (d). The entropy S is computed from ρ_m averaged over the time range $2^{23} \leq t \leq 2^{24}$ (blue-black $\circ$) and $2^{16} \leq t \leq 2^{17}$ [red-gray + in (a), (b)] or $2^{11} \leq t \leq 2^{12}$ [red-gray + in (c)]. The theory curves $S(E)$ for BE (red-gray) and EQ [blue-black in (a),(b),(c) or green in (d)] are from ρ_m values of [Eq. (2)] with E_m values of the used RMT realization (a), (b),(c) or a fictitious spectrum according to the semicircle law in (d) [where E_m is the solution of $m - 1/2 = M(E_m)$, $m = 1, \ldots, N$ with $M(E)$ being the integrated density of states].

given by the BE (or QG) ansatz. The quantities S and E are extensive (self-averaging), and it was argued that their analysis is more preferable as compared to the direct study of the strongly fluctuating probabilities ρ_m [36,37,39,40]. Here we show that the ergodicity of RMT eigenstates of $\hat{H}$ allows one to reduce significantly the fluctuations and to obtain stable results for ρ_m that are clearly described by the EQ ansatz [Eq. (2)].

The numerical integration of [Eq. (1)] is done with the symplectic scheme of order 4 [43–45] using a step size $\Delta t = 0.1$ up to maximal times $t = 4 \times 10^6 - 1.3 \times 10^8$ with exact norm conservation, energy conservation with accuracy $\sim 10^{-8}$, and for the GOE matrix size $N = 64$ (see the Supplemental Material [11] for more details and results for other values $N = 32$, 128, 256, 512). As initial condition, we choose an eigenmode $\phi_n^{(m)}$ of $\hat{H}$ at some index m (sometimes also noted m_0) such that the energy remains close to the initial energy $E \approx E_m$. Examples of the time dependence $S(t)$ are shown in the Supplemental Material [11], Fig. S1, demonstrating a steady-state regime reached at times $t > 10^4$ for $\beta = 1$. The obtained dependence $S(E)$ is shown in Fig. 1 at different β values for a specific RMT realization and two timescales and also for 10 RMT realizations at $\beta = 1$. At small values $\beta = 0.02$, 0.1 the system is close to an integrable KAM regime [7,8] while at $\beta = 1$ essentially all modes are thermalized (see Fig. 1, Fig. S2 in the Supplemental Material [11], and additional material in Ref. [46]). These results show that the critical border for thermalization is located at $\beta_c \sim 0.1$

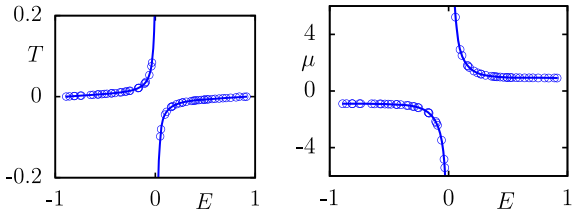

FIG. 2. Dependence of T and μ on energy E for EQ ansatz [Eq. (2)] (curves); data points are for $\beta = 1$, $N = 64$, and time range $2^{23} \leq t \leq 2^{24}$, with T and μ determined from norm and numerical entropy values [same RMT realization as in Fig. 1(c)].

independent of N. However, the exact determination of β_c is a rather complicated task due to the presence of many-body nonlinear effects like, e.g., the Arnold diffusion [7,8]. Also at the spectral borders $E \approx \pm 1$ the spacing between energies E_m increases according to the semicircle law [29], and therefore it is more difficult to reach thermalization there.

An important feature of Fig. 1 is that the theory curves $S(E)$ obtained with the BE and the EQ ansatz [Eq. (2)] are rather close to each other. Thus due to fluctuations of numerical data for $S(E)$ it is difficult to determine which theory BE or EQ better describes the numerical data. However, the data points are significantly closer to the BE curve, especially for moderate energies $|E| \approx 0.5$–0.8 where both curves are somewhat different [the difference between the QG and BE $S(E)$ curves, not visible on graphical precision, is ~ 0.003 at the spectral borders and much smaller at other E values, so that we discuss mainly the BE case].

For the EQ ansatz the dependencies $T(E)$, $\mu(E)$, obtained by the solution of the equations for energy and norm for a given RMT spectrum, are shown in Fig. 2 (the Supplemental Material [11], Fig. S3, for the BE ansatz) for the thermalized regime at $\beta = 1$. The numerical points obtained from E and norm values are by definition exactly located on the theory curves. If instead of E we use the numerical data of S then the points slightly deviate from the theory (Fig. 2 and Fig. S3 in the Supplemental Material [11]), but the T and μ values themselves are drastically different between BE and EQ cases.

The most direct way to distinguish between BE and EQ cases is to compare the probability dependence $\rho_m(E)$ with the theory [Eq. (2)]. Such a comparison is shown in Fig. 3 for four initial states at $m = m_0$, $\beta = 1$, and $N = 64$ (more data are in the Supplemental Material [11], Fig. S4, and Ref. [46]). The dynamical thermalization clearly follows the EQ ansatz and not at all the BE one, except for an initial state at $E_{m_0} \approx 0$ where both approaches are equivalent. This observation is in agreement with the classical statistical mechanics [4,42]. The probabilities ρ_m for all initial energies E_{m_0} are shown in Fig. 4 with a good agreement between the numerical data and the EQ ansatz (see Ref. [46] for figures such as Fig. 3 for all m_0 values).

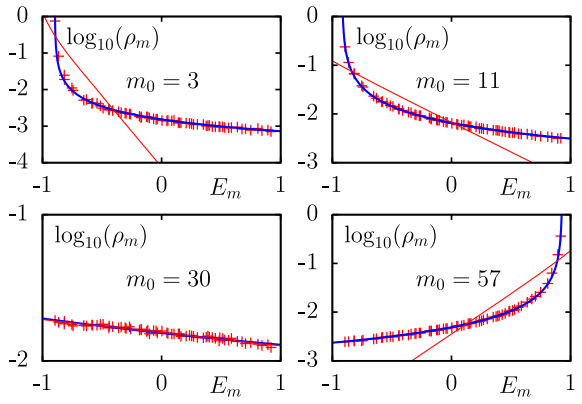

FIG. 3. Dependence of $\rho_m(E_m)$ on E_m for four initial states at $m_0 = 3$, 11, 30, and 57 with negative temperature $T < 0$; here $\beta = 1$, $N = 64$, and time average range $2^{23} \leq t \leq 2^{24}$. The blue curve shows the theory of EQ ansatz with $\rho_{\rm EQ}(E) = T/(E-\mu)$. The red line shows BE ansatz theory $\rho_{\rm BE}(E) = 1/(\exp[(E-\mu)/T]-1)$; T, μ theory [Eq. (2)] values are given in the Supplemental Material [11], Fig. S4, for BE and EQ cases.

The statistical distribution $p(x)$ of fluctuations of the rescaled quantity $x = (E_{m_0} - \mu)|C_m(t)|^2/T$ (with μ, T from the EQ ansatz for the energy E_{m_0}) also follows the Boltzmann law $p(x) = \exp(-x)$ (see the Supplemental Material [11], Fig. S5).

In Fig. 5 we show the energy dependence of the maximal positive Lyapunov exponent λ_m on energy E_m of initial state m for different β values (more data are in the Supplemental Material [11], Figs. S6–S10, and Ref. [46]). In the thermalized phase $\beta = 1$ we have a smooth variation of λ with E_m while below or close to the thermalization border at $\beta = 0.1$ high λ_m values appear only at specific E_m values. We attribute this to the existence of triplets of energies with very close E_m values. Indeed, in a hypothetic case of three equal E_m values the KAM theory is not valid and developed chaos exists at arbitrary small β values as is shown in Refs. [33,47]. Nonetheless, in RMT there is level repulsion, and double or triple degeneracies are forbidden leaving place only to quasidegeneracy of levels so that KAM becomes valid at $\beta \to 0$. Thus for $\beta = 0.02$ we have typically λ_m approaching to zero with increasing time. Our preliminary results show that in the thermal phase at larger $|T|$ (if $E_m \approx 0$) we have an approximate dependence $\lambda \sim \beta^{\eta}/N^{\nu}$ with $\eta \approx 1.52$, $\nu \approx 1.89$ (see the Supplemental Material [11], Figs. S6–S10). However, the Lyapunov exponent dependence on β and N requires further detailed studies.

Finally, we discuss the reasons why the nature of thermal equipartition, BE or EQ, was so difficult to establish in previous studies [36,37,39,40]. One of them is the proximity of $S(E)$ curves for both approaches. At the same time the direct determination of the $\rho_m(E)$ dependence is rather difficult due to significant fluctuations, as it was pointed out previously. These fluctuations are especially large for the DANSE case at a large disorder ($W = 4$ in Ref. [36]) when the localization length ℓ is significantly smaller than system size N ($\ell/N \approx 0.1$ at $N = 64$). We illustrate this in the Supplemental Material [11], Figs. S11–S12, showing that at smaller disorder $W = 2$ with larger localization length ℓ the fluctuations of ρ_m are reduced and at long times we have an agreement of $\rho_m(E)$ with the EQ ansatz and strong deviations from the BE ansatz. For the NLIRM model [Eq. (1)] the linear eigenmodes are ergodic, i.e., no localization, and the fluctuations of $\rho_m(E)$ are significantly reduced, which allows one to distinguish clearly between EQ and BE cases.

The cases of GPE in the Bunimivich stadium [39] and the Sinai-oscillator trap [40] are somewhat different. Indeed, in these models the spectrum of the linear system is unbounded so that, even if linear eigenstates are in the quantum chaos regime, the probability spreading to high energies is rather slow due to small coupling transitions induced by nonlinearity between states with significantly different energies. Thus in these systems there is a

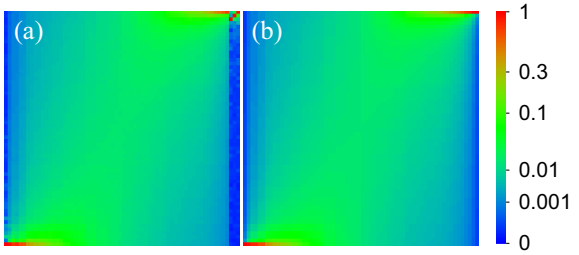

FIG. 4. Density plot of ρ_m for parameters of Fig. 3 with initial state index $1 \leq m_0 \leq 64$ in the x axis and $1 \leq m \leq 64$ in the y axis. The colorbar shows ρ_m values in a nonlinear scale to increase the visibility of small ρ_m values. (a) Numerical data for $\beta = 1$, $N = 64$. (b) The EQ ansatz $\rho_{\rm EQ}(E_m)$ (see also Fig. 3).

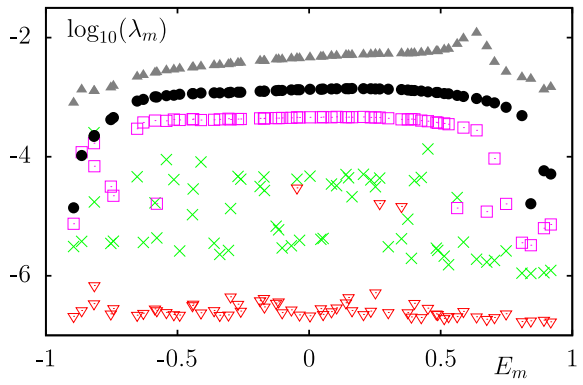

FIG. 5. Lyapunov exponent λ_m dependence on E_m with m being the index of the initial state for $N = 64$; λ_m is determined from the fit $\ln \|\Delta\psi(t)\| = a + b\ln(t) + \lambda_m t$ for $\beta = 2$ (gray triangle, top); 1 (black circle); 0.5 (pink square); 0.1 (green cross) at $t \leq 2^{22}$; $\beta = 0.02$ for $t \leq 2^{27}$ (red $\triangledown$, bottom).

formation of a relatively compact probability packet at low energies which spreads to high energies very slowly in time. Such an energy packet of ρ_m gives $S(E)$ values compatible with the curve of the BE ansatz; however the fluctuations of $\rho_m(E)$ are very strong with a significant difference from the BE distribution at high energies (see, e.g., Fig. 5 in Ref. [39] and Figs. 8 and 11 in Ref. [40]). To analyze these features in more detail, we add to the diagonal RMT matrix element $H_{n,n}$ an additional diagonal energy fn with a constant $f > 0$. Then the variation of linear energies fN becomes rather large and exceeds significantly those of the RMT case. The results for this model at $\beta = 1$, $f = 0.25$ show that at times $t = 2^{15}$ for $N = 32$ (or $t = 2^{20}$ for $N = 64$) the probabilities $\rho_m(E)$ form a compact packet of approximate BE shape and the EQ thermal distribution is reached (with fluctuations) only at very large times $t = 2^{27}$ (see the Supplemental Material [11], Figs. S13 and S14). Such large timescales were out of reach in Refs. [39,40] due to the complexity of the numerical integration of GPE.

In conclusion, we showed that a nonlinear perturbation of RMT leads to dynamical thermalization with energy equipartition corresponding to the laws of classical statistical mechanics [4,42]. Such a thermalization appears due to dynamical chaos in finite systems with a moderate or large number of degrees of freedom at weak or moderate perturbation of a linear RMT system. At very weak perturbations the system dynamics is characterized by a quasi-integrable KAM regime. We argue that the proposed NLIRM model captures the generic features of dynamical thermalization in systems weakly perturbed by classical nonlinear fields and does not depend on the specific form of the nonlinear term (see detailed discussion in the Supplemental Material [11] and Figs. S15 and S16 there). Of course, for finite many-body quantum systems with second quantization the interactions lead to quantum dynamical thermalization and distributions of Bose-Einstein for bosons or Fermi-Dirac for fermions, as has been demonstrated in numerical studies [48] and Refs. [49–51] respectively.

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Note added.—After submission of this work a dynamical thermalization at negative temperature in EQ [Eq. (2)] has been observed in optical fibers [52]. See also the discussion in the Supplemental Material [11].

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