Dynamical Thermalization of Disordered Nonlinear Lattices

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We study numerically how the energy spreads over a finite disordered nonlinear one-dimensional lattice, where all linear modes are exponentially localized by disorder. We establish emergence of dynamical thermalization, characterized as an ergodic chaotic dynamical state with a Gibbs distribution over the modes. Our results show that the fraction of thermalizing modes is finite and grows with the nonlinearity strength.

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The studies of ergodicity and dynamical thermalization in *regular* nonlinear lattices have a long history initiated by the Fermi-Pasta-Ulam problem [1] but they are still far from being complete (see, e.g., [2] for thermal transport in nonlinear chains and [3] for thermalization in a Bose-Hubbard model). In this Letter we study how the dynamical thermalization appears in nonlinear *disordered* chains where all linear modes are exponentially localized. Such modes appear due to the Anderson localization, studied since fifty years in the context of electron transport in disordered solids [4]. Such a localization is a general phenomenon describing various physical situations [5, 6]. Examples beyond the initial Anderson formulation are wave propagation in a random medium [7], localization of a Bose-Einstein condensate [8] and quantum chaos [9]. In simple terms, localization means that in a linear disordered system in one and two dimensions, for almost all random realizations of the potential the eigenstates are exponentially localized and the spectrum is pointlike [5]. It manifests itself as a vanishing mobility of electrons, an exponentially small transparency of a random layer for waves, and a suppression of classical diffusion for quantum chaos.

Effects of nonlinearity on localization properties have attracted large interest recently. Indeed, nonlinearity naturally appears for localization of a Bose-Einstein condensate, as its evolution is described by the nonlinear Gross-Pitaevskii equation [10]. An interplay of disorder, localization, and nonlinearity is also important in other physical systems like wave propagation in nonlinear disordered media [11, 12] and chains of nonlinear oscillators with randomly distributed frequencies [13].

The main question here is whether the localization is destroyed by nonlinearity. It has been addressed recently using two physical setups. In refs. [14, 15]it has been demonstrated that an initially concentrated wavepacket spreads apparently indefinitely, although subdiffusively, in a disordered nonlinear lattice, provided the nonlinearity is strong enough. Also at consideration of a transmission through a nonlinear disordered layer [16, 17] it has been demonstrated that chaotic destruction leads to a drastically enhanced transparency.

Here we study thermalization properties of the dynamics of a nonlinear disordered lattice – discrete Anderson nonlinear Schrödinger equation (DANSE). We describe in details the features of the evolution, in a finite lattice, of an initially localized excitation toward a statistical equilibrium. We demonstrate that already this equilibrium is nontrivial due to existence of two conserved quantities, the energy and the total probability. Moreover, we find non-thermalizing modes and characterize their dependence on the nonlinearity and the lattice length.

We model a nonlinear disordered medium by DANSE model:

$$i\frac{\partial \psi_n}{\partial t} = E_n\psi_n + \beta|\ \psi_n\ |^2\psi_n + \psi_{n+1} + \psi_{n-1}\ , \quad (1)$$

where β characterizes nonlinearity, and the on-site energies E_n (or frequencies) are independent random variables distributed uniformly in the range $-W/2 < E_n < W/2$ (they are shifted in such a way that $E = 0$ corresponds to the central energy of the band). We consider a finite lattice $1 \le n \le N$ with periodic boundary conditions. Then DANSE is a classical dynamical system with the Hamilton function

$$H = \sum_n E_n|\psi_n|^2 + \psi_{n-1}\psi_n^* + \psi_{n-1}^*\psi_n + \frac{\beta}{2}|\psi_n|^4\ . \quad (2)$$

It exactly describes recent experiments with one-dimensional nonlinear photonic lattices (cf. Eq. (1) in [12]), and also serves as a paradigmatic model for a wide class of physical problems where interplay of nonlinearity and disorder is important.

For $\beta = 0$ all eigenstates are exponentially localized with the localization length $l \approx 96W^{-2}$ (for weak disorder) at the center of the energy band [6]. Below we mainly focus on the case of moderate disorder $W = 4$, for which $l \sim 6$ at the center of the band and $l \approx 2.5$ at $E = \pm 2$. For each particular realization of disorder a set of eigenergies ϵ_m and of corresponding eigenmodes φ_{nm} can be found. In this eigenmode representation

$\psi_n = \sum C_m \varphi_{nm}$ the Hamiltonian reads

$$H = \sum_m \epsilon_m |C_m|^2 + \beta \sum_{klji} V_{klji} C_k C_l C_j^* C_i^* , \qquad (3)$$

with $\sum_m |C_m|^2 = 1$, and $V_{mm'm_1m_1'} \sim l^{-3/2}$ are the transition matrix elements [18]. This representation is mostly suitable to characterize the spreading of the field over the lattice, since in this basis the transitions take place only due to nonlinearity. Moreover, in the mode representation one can see that the nonlinear contribution to the energy is in fact small even if β is of order of one: as it follows from (3), this contribution is $\sim \beta/l$ if only one mode is excited.

To study the dynamical thermalization in a lattice, we performed direct numerical simulation of DANSE (1), using mainly two methods: the unitary Crank-Nicholson operator splitting scheme with step $\Delta t = 0.1$ as described in [15], and a 8-order Runge-Kutta integration with step $\Delta t = 0.02$; in both cases the total energy and the normalization have been preserved with high accuracy. We started with two types of localized initial states: (A) one site seeded, i.e. $|\psi_n(0)|^2 = \delta_{n,j}$ and (B) one mode initially excited, i.e. $|C_m(0)|^2 = \delta_{m,k}$. For different realizations of disorder, we seeded different possible sites/modes and followed the evolution of the field solving (1) up to times (in selected runs) $\sim 10^8$. The level of spreading is characterized by the entropy of the mode distribution

$$S = -\sum_m \rho_m \ln \rho_m \ , \qquad \rho_m = \overline{|C_m|^2} \ , \qquad (4)$$

where overline means time averaging. For one excited mode $S = 0$ while $S = \ln N$ for a uniform distribution over all modes in a lattice of length N. To give an impression of a time evolution of the thermalization process we show in Fig. 1 several time dependencies of the entropy (4). The time averaging has been performed over doubling time intervals (i.e. over the time intervals between successive markers in this figure which are periodic on a logarithmic time scale). One can see that for the setup (B) some modes remain localized for all times (cf. [19]), while other after some transient time evolve to a state with large entropy. For the setup (A), in all situations the entropy grows and saturates at a certain level. In our discussion below we focus therefore on the setup (B) as on mostly nontrivial one.

The crucial issue is that, because of the conservation of the total energy and of the total probability, the thermalization generally cannot lead to an equipartition between all modes. To derive an approximate expression for the statistically stationary distribution ρ_m, we mention that it should satisfy $\sum \rho_m = 1$ and $E = \sum \rho_m \epsilon_m$, where, in view of discussion above, we have neglected the nonlinear contribution to the energy. Then the condition of maximal entropy (4) leads, after a standard calculation, to a

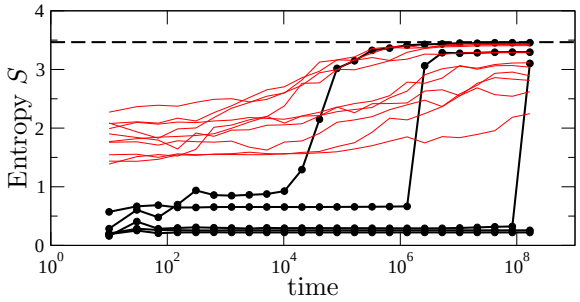

FIG. 1: (color online) Time evolution of entropy S (4) in DANSE (1) with $N = 32$ and $\beta = 1$, for a particular realization of disorder and different initial states: bold black curves with markers – single-mode initial states (B) with energies $E = -0.34, 0.76, -0.29, 3.36, -0.5$ (curves from top to bottom at $t = 10^8$, two bottom cases are very close), solid red/gray curves – single-site initial states (A, ten randomly chosen states). The dashed line shows the level $S = \ln 32$.

Gibbs distribution

$$\rho_m = Z^{-1} \exp(-\epsilon_m/T), \qquad Z = \sum_m \exp(-\epsilon_m/T). \quad (5)$$

Here T is an effective "temperature" of the system, induced by dynamical chaos. The entropy and the energy are related to each other via usual expressions [20]

$$E = T^2 \partial \ln Z/\partial T \ , \qquad S = E/T + \ln Z \ . \qquad (6)$$

This value of entropy yields the maximal possible equipartition for the given initial energy, and the values of Fig. 1 obtained via a numerical simulation of the disordered nonlinear lattice, should be compared with the values from the Gibbs distribution. Because we have anyhow neglected the effects of nonlinearity in the theoretical value of the entropy, we adopt other simplifications: approximate the density of states of the disordered system as a constant in an interval $-\Delta < \epsilon < \Delta$ and consider the eigenenergies ϵ_m in a particular realization of disorder as independent random variables distributed according to this density. Also we assume the variations of the partition sum to be small and use $\langle \ln Z \rangle \approx \ln \langle Z \rangle$, where brackets denote averaging over disorder realizations. In this approximation we obtain

$$\langle \ln Z \rangle \approx \ln N + \ln \sinh(\Delta/T) - \ln(\Delta/T). \qquad (7)$$

At $W = 4$ we have $\Delta \approx 3$ (see Figs. 3,5 below) and this theory gives the dependence $S(E)$ within a few percent accuracy compared to S averaged over disorder within Gibbs computations with exact numerical values ϵ_m. We note that $T = +0, \pm\infty, -0$ correspond to $E = -\Delta, 0, +\Delta$ respectively (as in the standard two-level problem, see related discussion in [20]).

We compare in Fig. 2 the Gibbs distribution (5) with the results of direct numerical simulations of DANSE using N_d disorder realizations. Here we present the values

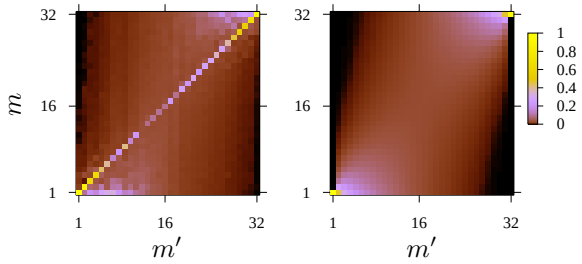

FIG. 2: (color online) Left: time and disorder averaged probability $\langle\overline{\rho_m(m')}\rangle$ in mode m for initial state in mode m'. Right: theoretical values according to the Gibbs distribution (5). Here $N = 32, \beta = 1, N_d = 15$.

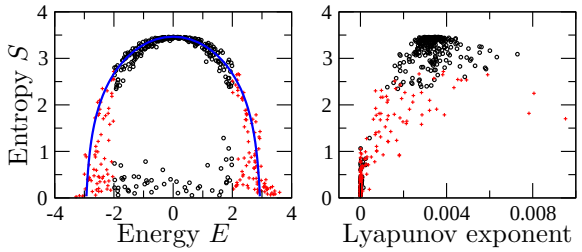

FIG. 3: (color online) Left panel: Final entropies (4) after an evolution during time interval 10^7, averaged over a time interval of 10^6. The states evolving from initial modes in the middle of the band (see text) are marked with circles, and those at the edges of the band by pluses; the curve shows the approximate theory (7). Right panel: Lyapunov exponents (averaged over a time interval 10^6) vs. entropy for the same sets. Here $N = 32$, $\beta = 1, N_d = 7$.

$\langle\overline{\rho_m}\rangle$ averaged over time and over different realization of disorder, in dependence of the number of initially seeded mode m'. The modes have been ordered according to their energy, so that $m = 1$ corresponds to the maximal energy. One can see a good correspondence between the numerics and the simple theory (5) with one crucial discrepancy: the peaks on the diagonal $m = m'$ indicate that there are cases when there is no thermalization and the energy remains in the initially seeded mode.

To characterize thermalized and non-thermalized cases quantitatively, we compare in Fig. 3 numerical values for the entropy according to Eq. (4) with the theoretical Gibbs computation given by Eqs.(5,6,7). Clearly, the Gibbs theory gives a satisfactory global description of numerical data. The nonthermalized modes in this presentation are those at the bottom of the graph; these states are absent for the setup (A) where initial sites are seeded.

It appears appropriate to discuss the dynamics of the modes in the middle of the energy band and at the edges separately. Roughly, one can attribute modes with energies $-2 < \epsilon_m < 2$ to the former and modes with $|\epsilon_m| > 2$ to the latter class. For the modes in the middle of the energy band the maximal entropy according to (6) is close to $\ln N$, and one clearly distinguishes the thermalized modes and those that remain localized, as those reaching the maximal entropy and those remaining at the level $S \lesssim 1$, correspondingly.Thermalization is associated with the chaotic dynamics of the DANSE lattice. To demonstrate this, we calculated the largest Lyapunov exponents λ shown in Fig. 3 (right panel) for the states with entropies shown on left panel. One can see that all modes with $S < 1$, i.e. those that do not thermalize, have nearly vanishing λ, while in the thermalized states ($S > 2$) the positive values of λ clearly indicate for chaos.

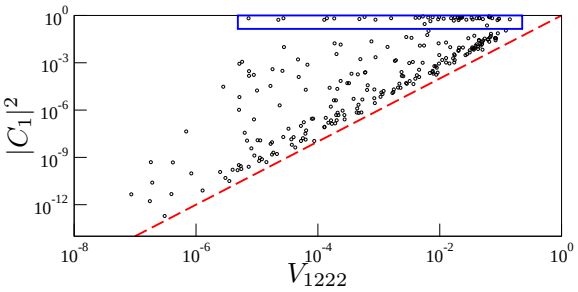

FIG. 4: (color online) Average probability of the mode $m = 1$ vs. the coupling matrix element V_{1222}; only the mode $m = 2$ is excited initially. Here $N = 32, \beta = 1$. The blue box shows the cases of thermalization, where the mode $m = 1$ reaches energy comparable with that of $m = 2$. In all other cases the energy in the mode $m = 1$ is exponentially small. The dashed red line $|V_{1222}|^2$ gives the lower bound.

The above distinction between thermalized and non-thermalized states is less evident for modes at the band edges (shown by red/gray pluses in Fig. 3). Here already the theoretical value of entropy given by Eqs. (5,6,7) is rather small. Hence, the spreading can go only over a few "available" modes only. Nevertheless, also here one can see from Fig. 3 a clear correlation between the entropy and the Lyapunov exponent. Moreover, in several cases the Lyapunov exponent at the edge of the spectrum is definitely larger than in the middle. This happens because the energy spreads over a small number of modes, the effective nonlinearity is larger because the amplitude of each mode is large, and therefore chaos is stronger.

In the discussion above we did not account for a spatial organization of the mode structure. The latter is less important for the modes in the middle of the band, where one can expect always to find neighbors with a close energy. Contrary to this, for the energies at the edges the issue of spatial distance becomes essential. Indeed, since here the thermalization is possible only over a few modes, it is important whether these modes are spatially separated or not. For the eigenmodes m and m' at $\beta = 0$ the natural measure of this separation is the coupling matrix element $V_{m'm'm'm}$ according to (3). This coupling is exponentially small for spatially separated modes due of their localization. One can expect, that a mode at the edge of the spectrum will be thermalized only if the distance to other few modes in the lattice with a close energy is small (i.e. if V is large). To check this, we have performed the following computation: for different real-

izations of disorder, we seeded the mode with the second lowest energy in the spectrum, and looked if in course of the dynamical evolution the mode with the lowest energy will be excited. These two modes are close in energy, but may have large spatial separation resulting in the small coupling constant. The results of this analysis are presented in Fig. 4. One can see that the first mode is not excited unless the coupling constant to the second mode is large enough. But even in this case, an effective excitation occurs only in a small fraction of realizations (40 out of 256).

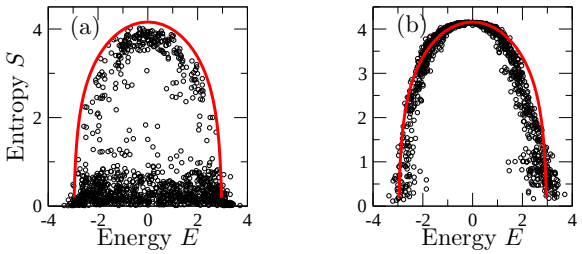

FIG. 5: (color online) Dependence of entropy S on energy E as in Fig. 2 but for $N = 64, N_d = 18$, and two values of nonlinearity: (a) $\beta = 0.5$, (b) $\beta = 2$. Averaging have been performed over the time interval 10^6 after an initial evolution during time 10^6; for small β still longer times are needed to reach thermalized state with maximal S at given E.

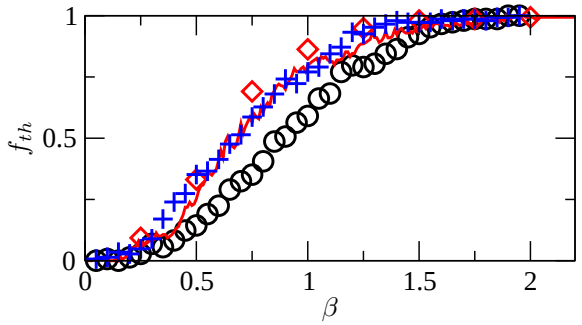

FIG. 6: (color online) A fraction of thermalized (after time 10^6) modes f_{th} from the middle of the band as a function of nonlinearity β for $N = 16$ (circles), 32 (bold line), and 64 (pluses). Several values for time 10^7 and $N = 32$ are shown with diamonds.

Finally, we discuss how the thermalization properties depend on the nonlinearity constant β. In Fig. 5 we show the dependence $S(E)$ for different nonlinearities β. For $\beta = 0.5$ a large portion of the initial states remains non-thermalized, while for $\beta = 2$ all states are thermalized (at least in the sense that their entropy is close to the maximal possible one, as discussed above this is a good criterion in the middle of the band). To determine how the fraction of thermalized states depends on nonlinearity β we use the following procedure. For the initial modes in the middle of the band (i.e. for $|E| < 2$) we classified those that reach the entropy more than the half of the maximal value (i.e. the level $\ln(N)/2$) as thermalized, and those that remain below this level as non-thermalized. The fraction f_{th} of the thermalized modes, shown in Fig. 6, monotonously increases with β. At fixed β the numerical data indicate saturation of f_{th} at large N, but more detailed checks at longe sizes and longer times are required. For example, recent results on self-induced transparency of a disordered nonlinear layer [17] show decrease of critical β with lattice size for $N \leq 32$.

Our main conclusion is that the maximally thermalized state, that emerges as a result of chaotic dynamics, is described by the Gibbs distribution over the linear modes, with some effective *temperature*, depending on the initial excitation. Not all modes lead to thermalization, some fraction of them remains localized, but this fraction decreases with nonlinearity. Further studies are still required to establish the properties of this thermalization, in dependence on the nonlinearity strength, on the disorder properties, and on the lattice size.

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