Simple statistical explanation for the localization of energy in nonlinear lattices with two conserved quantities

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The localization of energy in the discrete nonlinear Schrödinger equation is explained with statistical methods. The partition function and the entropy of the system are computed for low-amplitude initial conditions. Detailed predictions for the long-time solution are derived. Localized high-amplitude excitations absorb a surplus of energy when they emerge as a by-product of the production of entropy in the small fluctuations. The thermodynamic interpretation of this process applies to many dynamical systems with two conserved quantities.

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Localization of energy within a small number of isolated high-amplitude structures is a widespread phenomenon in nonlinear optics [1–3], plasma physics [4], Bose-Einstein condensates [5], and nonlinear lattice dynamics [6–8,10]. Peaks of the energy density result either from a collapsing wave train that leads to a finite-time blow-up of the amplitude [4,11], or, in spatially discrete systems, from a sequence of merging breathers [8].

The purpose of this paper is to show that the formation of peaks is driven by the production of entropy and that this behavior is generic for the thermalization of many conservative systems where a second quantity is conserved in addition to the Hamiltonian. The discrete nonlinear Schrödinger equation is a simple generic equation that describes discrete breathers in nonlinear optical waveguide arrays [2,3] and dilute Bose-Einstein condensates that are trapped in periodic potentials [5]. The spatial discreteness avoids the leakage of energy to infinitesimal scales that can occur during the wave collapse of continuous systems [9] so that this system is a simple but representative model for localization processes. The noncompactness of the phase space leads to a merely technical difficulty in the statistical treatment of high-amplitude structures.

Figure 1(a) shows the focusing process for the focusing discrete nonlinear Schrödinger equation (DNLS)

$$i\dot{\phi}_n = \phi_{n+1} + \phi_{n-1} + |\phi_n|^2 \phi_n . \tag{1}$$

Any coefficients of this equation can be removed by scaling, and consequently all quantities are dimensionless. First, breathers with moderate amplitudes appear periodically in space and time following a phase instability of a regular low-amplitude initial solution. Subsequently, they merge into more persistent peaks with higher amplitudes [lattice site 188 in Fig. 1(a)]. The system finally settles into a state where immobile high-amplitude peaks [the ring with $|\phi| \approx 2.3$ in Fig. 1(b)] emerge from a low-amplitude disordered background (core with $|\phi| < 0.5$). The peaks divide the system into patches of the order of 100 lattice sites where the amplitude is low and the dynamics is irregular. The peaks oscillate corresponding to their amplitude-dependent frequency and their amplitudes fluctuate slightly, but their position in the lattice almost never changes.

This behavior depends crucially on the system's energy $E = \langle \mathcal{H} \rangle$, where $\mathcal{H} = \Sigma_i (\phi_i \phi_{i+1}^* + \phi_i^* \phi_{i+1}) + \frac{1}{2} \phi_i^2 \phi_i^{*2}$ is the Hamiltonian of the DNLS $i\dot{\phi}_n = \partial \mathcal{H} / \partial \phi_n^*$. Persistent localization of energy occurs only if the system's energy is positive. In this case the peaks finally absorb almost the total energy [Fig. 2(a)]. The height of the peaks $|\phi| \approx 2, \ldots, 2.5$ is almost independent of the total energy [Fig. 2(b)], but the number of peaks increases with the energy. For negative energies, there is no localization of energy [Fig. 1(c)] and the system settles into a state of low-amplitude fluctuations [Fig. 1(d) and Fig. 2(a)]. The system's second conserved quantity, the modulus-square norm (or "particle number") $A = \langle \mathcal{A} \rangle$

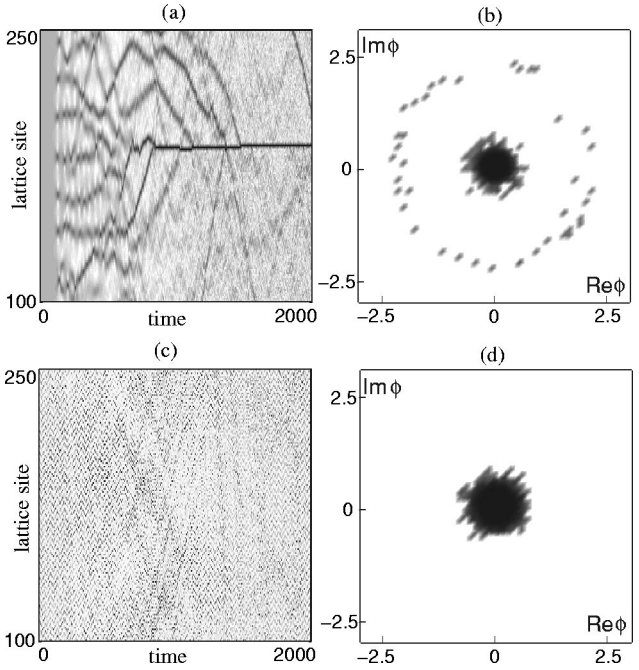

FIG. 1. Numerical integration of the DNLS with 4096 oscillators. The initial conditions are waves with the amplitude $\phi_n = 0.3$ and the wave number $k = 0$ for (a), (b), and with $k = \pi/2$ for (c), (d). (a) and (c) show the spatiotemporal patterns of high-amplitude states (dark gray) in a small sector of the chain for the first 2000 time steps. (b) and (d) show the distributiions of ϕ after 2×10^5 time steps.

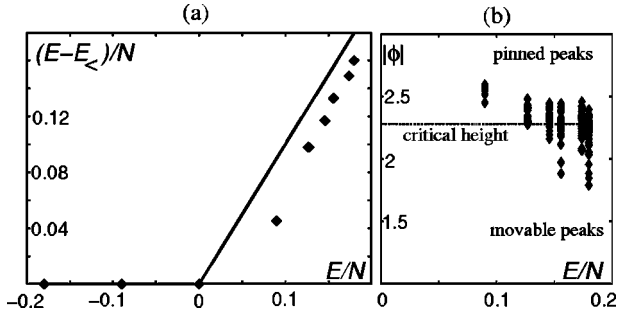

FIG. 2. Energy [dots in (a)] and height [dots in (b)] of peaks with $|\phi|>1$ as a function of the total energy after 2×10^5 time steps of numerical integration. The initial conditions of the 4096 lattice sites are waves with an amplitude $|\phi|=0.3$ and wave numbers from $k=0$ to $k=\pi$. Lines, thermodynamic equilibrium value (a) and critical height for lattice pinning (b).

with $\mathcal{A}=\Sigma\phi_i\phi_i^*$ is also crucial for this phenomenon. There is no persistent localization of energy in this system if the rotational symmetry linked to this second conserved quantity is broken.

The discrete nonlinear Schrödinger equation admits energies $-2A\leqslant E\leqslant 2A$ for low-amplitude initial conditions $A/N\ll 1$. As suggested by Fig. 1(b), the phase space may be separated into a low-amplitude domain $\Delta_<$ for $|\phi_<|<r$ and a high-amplitude domain $\Delta_>$ for $|\phi_>|\geqslant r$. To avoid formal difficulties with diverging terms, a preliminary upper bound $R>r$ of the phase space is introduced as $|\phi|\leqslant R$. The main contributions to the energy arise from interactions in the low-amplitude domain (where $N-K$ oscillators are gathered and nonlinear contributions are negligible) and from the quartic contribution of $K\ll N-K$ oscillators in the high-amplitude domain. The Hamiltonian is therefore approximated as

$$\mathcal{H}\approx\mathcal{H}_<+\mathcal{H}_>=\sum u(r-|\phi_i|)u(|r-|\phi_{i+1}|)\times(\phi_i\phi_{i+1}^*+\phi_i^*\phi_{i+1})+\frac{1}{2}u(|\phi_i|-r)\phi_i^2\phi_i^{*2} \quad (2)$$

with the unit step function $u(x<0)=0$, $u(x\geqslant 0)=1$. The second integral of motion may be separated in a similar way as $\mathcal{A}=\mathcal{A}_<+\mathcal{A}_>$. The system's entropy as a function of the conserved quantities E and A can be computed from the grand partition function $y(\beta,\gamma)=\int\rho\Pi_{i=1}^N d\phi_i d\phi_i^*$ using the density $\rho=e^{-\beta(\mathcal{H}-\gamma\mathcal{A})}$. The partition function is a sum over all possible numbers of peaks K, and only its leading term

$$y(\beta,\gamma)\approx\binom{N}{K}y_<(\beta,\gamma,N-K)y_>(\beta,\gamma,K) \quad (3)$$

will be considered. K and R will be determined later in order to maximize the entropy. The factor $\binom{N}{K}$ gives the number of combinations of K high-amplitude sites on N lattice sites. The contributions $y_<$ and $y_>$ will be computed separately. The patches of small-amplitude fluctuations between the peaks give the contribution

$$y_<(\beta,\gamma)=\int_{\Delta_<}\cdots\int_{\Delta_<}\rho_<\prod_{i=1}^{N-K}d\phi_i d\phi_i^* \quad (4)$$

to the partition function with $\rho_<=e^{-\beta(\mathcal{H}_<-\gamma\mathcal{A}_<)}$. These regions are in thermal equilibrium with each other, and therefore they are regarded as one single field of $N-K$ oscillators. Similarly, the K oscillators in the high-amplitude regime $\Delta_>$ have degrees of freedom corresponding to variations of phase and amplitude of the peaks. This leads to the contribution to the partition function

$$y_>(\beta,\gamma)=\int_{\Delta_>}\cdots\int_{\Delta_>}\rho_>\prod_{j=1}^{K}d\phi_j d\phi_j^* \quad (5)$$

with $\rho_>=e^{-\beta(\mathcal{H}_>-\gamma\mathcal{A}_>)}$. This neglects the coupling term of the peaks which is small compared to the quartic energy. However, peaks and fluctuations are coupled thermally, so that they can exchange energy and particles. This exchange vanishes on average when peaks and fluctuations have the same temperature β^{-1} and chemical potential γ. The energy $E\approx E_<+E_>$ and the particle number $A=A_<+A_>$ have contributions from either domain. A, $A_<$, $A_>$, $E_>$ are positive, E and $E_<$ may be positive or negative.

The partition function $y_<$ can be reduced to Gaussian integrals. The density may be written as $\rho_<=\Pi e^{-(\lambda_1\phi_n'-\lambda_2\phi_{n+1}')^2}e^{-(\lambda_1\phi_n''-\lambda_2\phi_{n+1}'')^2}$ with $\lambda_{1/2}=[\sqrt{-\beta(\gamma+2)}\pm\sqrt{-\beta(\gamma-2)}]/2$ (it turns out later that $-\beta\gamma\geqslant 0$ and $|\gamma|\geqslant 2$). Introducing the variables $x_n=\lambda_1\phi_n'-\lambda_2\phi_{n+1}'$, the partition function of the fluctuations is reduced to Gaussian integrals

$$y_<(\beta,\gamma)=\left(\int e^{-x_n^2}\det(\partial\phi_n'/\partial x_n)\prod dx_n\right)^2. \quad (6)$$

Using $\det(\partial x_n/\partial\phi_n')=\lambda_1^{N-K}-\lambda_2^{N-K}$, the Jacobian is $\det(\partial\phi_n'/\partial x_n)\approx\lambda_1^{-(N-K)}$ for $N-K\gg 1$ since $\lambda_1>\lambda_2$. The square in Eq. (6) is obtained from the identical integration over ϕ''. This gives an analytic expression for the partition function $y_<(\beta,\gamma,N-K)=\Lambda^{N-K}$ with $\Lambda=\pi\lambda_1^{-2}=\pi(-\beta\gamma+\sqrt{\beta^2(\gamma^2-4)})^{-1}$. The corresponding energy is

$$E_<=\left(\frac{\gamma}{\beta}\frac{\partial}{\partial\gamma}-\frac{\partial}{\partial\beta}\right)\ln y_<=(N-K)\frac{\sqrt{\gamma^2-4}-\sqrt{\gamma^2}}{\beta\sqrt{\gamma^2-4}} \quad (7)$$

and their particle number is

$$A_<=\frac{1}{\beta}\frac{\partial}{\partial\gamma}\ln y_<=-(N-K)\frac{\gamma}{\beta\sqrt{\gamma^4-4\gamma^2}}. \quad (8)$$

Consequently, the inverse temperature is $\beta=-2E_<(N-K)/(4A_<^2-E_<^2)$ and the chemical potential is $\gamma=(4A_<^2+E_<^2)/(2E_<A_<)$. Using these expressions, the canonic transformation $S_<=\ln y_<+\beta(E_<-\gamma A_<)$ leads to the entropy of the small fluctuations

$$S_<=(N-K)\ln\Omega \quad (9)$$

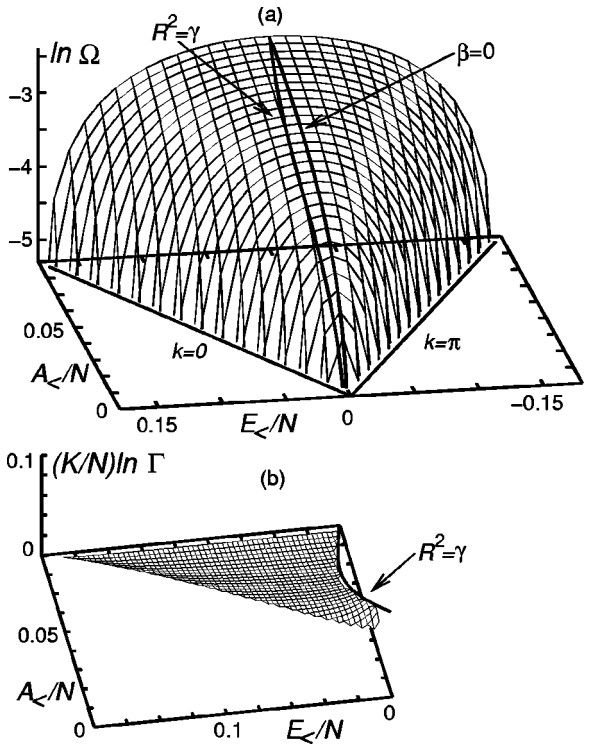

FIG. 3. $\ln\Omega$ (a) and $(K/N)\ln\Gamma$ (b) as a function of $E_<$ and $A_<$; line $R^2=\gamma$ for the simulation of Figs. 1(a) and 1(b).

with $\Omega=(4A_<^2-E_<^2)/[4A_<(N-K)]$. The entropy is the most useful thermodynamic potential in this context because its variables (particle number and energy) are known from the initial conditions. The fluctuation entropy per lattice site $\ln\Omega$ is plotted in Fig. 3(a). The lines $E_<=2A_<$ and $E_<=-2A_<$ correspond to waves with $k=0$ and $k=\pi$, respectively. The entropy is infinitely low for these ordered states. The ridge $E_<=0$ corresponds to a fluctuating state with an infinite temperature where all wave numbers have the same power. A wave with $k=\pi/2$ is a nonthermalized solution with $E=0$. This line $\beta=0$ was first computed in Ref. [7] where the additional nonlinear correction were included, and it was identified as the transition line to the localization phase. No analytic results for the statistics beyond this line have been available yet.

Equation (9) gives a valid expression for the total entropy if the system's total energy is negative [corresponding to the right slope with $E_<<0$ of Fig. 3(a)]. The temperature is positive in this case, and consequently the density $\rho_>\sim\exp(-\beta\Sigma|\phi_n|^4/2)$ decays rapidly for huge amplitudes so that the high-amplitude contribution to the partition function is negligible. In this phase only small fluctuations contribute to the total entropy $S=N\ln\Omega$. This describes the low-amplitude fluctuating state $(E=E_<,A=A_<)$ with no peaks of Fig. 1(d).

The slope $E_<>0$ is linked to negative temperatures [7]. The density $\rho_>$ increases with the amplitude in this regime which was suggested to be the reason for the formation of high-amplitude structures [7]. The increase of the density causes obvious technical difficulties. The phase space is (unlike in the spin system of Refs. [8,10]) noncompact, so that the integral $y_>$ will diverge for any fixed negative values of β. However, the artificial upper boundary R of the phase space prevents this divergence. The partition function can first be computed as a function of this parameter R, which subsequently will be allowed to go to infinity as this maximizes the entropy. From this the contributions of the peaks to the entropy, the energy, and the particle number can be computed.

The grand partition function of the peaks increases as $y_>(\beta,\gamma)\sim[e^{-\beta(R^4/2-\gamma R^2)}/(-\beta R^2+\beta\gamma)]^K$ with the cutoff R of the phase space if R is greater than $\sqrt{\gamma}$. Since the density ρ gathers at the border R, the particle number related to the domain $\Delta_>$ is $A_>=KR^2$ and the energy is $E_>=KR^4/2$. Inserting β, γ, and $R=\sqrt{2E_>/A_>}$ into the entropy of the peaks $S_>\approx -K\ln(-\beta R^2)$ yields

$$S_>=K\ln\left(\frac{K(4A_<^2-E_<^2)}{4(N-K)A_>E_<}\right)=K\ln(K/N)+K\ln\Omega+K\ln\Gamma \tag{10}$$

with $\Gamma=2A_<N/A_>E_<$. The combinations of $K=A_>^2/2E_>$ peaks on N lattice sites yield an entropy contribution $S_p=\ln\binom{N}{K}\approx K\ln(N/K)$. Adding up $S_<$, $S_>$, and S_p, the total entropy is

$$S=N\ln\Omega+\frac{A_>^2}{2E_>}\ln\Gamma. \tag{11}$$

This expression describes the thermodynamics in the domain where localization occurs. The small fluctuations provide the leading term $N\ln\Omega$ of the entropy while the contribution $K\ln\Gamma$ [Fig. 3(b)] from the peaks is negligible under the constraint $R^2>\gamma$ or $2E_>/A_>>(4A_<^2+E_<^2)/(2E_<A_<)$. $y_>$ and Γ can be computed in the same way for various types of nonlinearities. The entropy increases with $A_<$ and decreases with $|E_<|$ and has its maximum at $E_<=0$, $A_<=A$, $E_>=E$, $A_>=0$. The state of maximum entropy is related to low-amplitude fluctuations with $\beta=0$ and $\beta\gamma=-N/A$.

The crucial point is that the high peaks contribute little to the total entropy, while they can absorb high amounts of energy using only few particles. On the other side, the fluctuations can reach a state with a maximum entropy, if they contain the ideal amount of energy. This shows the thermodynamical nature of energy localization. In order to maximize the system's total entropy, the ideal amount of energy $E_<$ must be allocated to the fluctuations. Starting from an initial condition with a positive energy $E=E_<$ at the left slope in Fig. 3(a), the entropy can be increased when $E_<$ decreases while the released energy is stored in the localized structures. The state of maximum entropy corresponds to only one peak which absorbs the total energy [Fig. 2(a)] while consuming very few particles. This also shows the self-consistency of the truncation (2) that neglects the interaction of the peaks with their environment. The equilibrium state with localized structures corresponds to $\beta=0$, so the temperature is not negative. In the opposite case with nega-

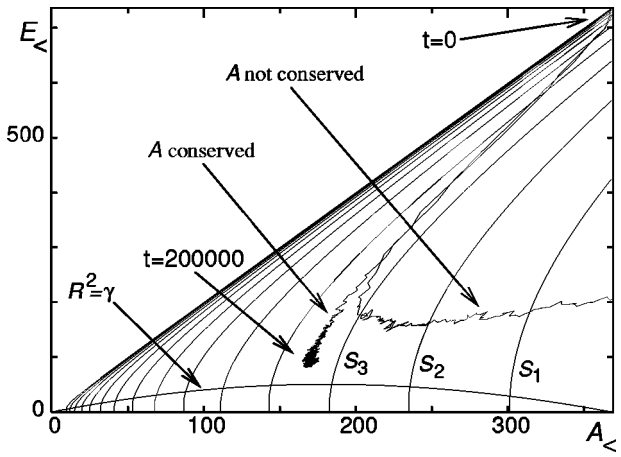

FIG. 4. Isentropes $S_1>S_2>S_3>\cdots$ for the left slope of Fig. 3(a); trace $(E_<,A_<)$ of the integration of Figs. 1(a) and 1(b) over $E_<$, $A_<$; trace for a version of the DNLS where the second conservation law is violated.

tive total energies E and a positive temperature, there is no energy surplus and consequently no localization [Figs. 1(c) and 1(d)]. Figure 4 gives a numerical picture of the shift of energy and particles into the peaks for Eq. (1) and the corresponding picture for a version of the DNLS where the rotational symmetry is broken by a small term $0.015\,\mathrm{Re}(\phi_n)$. It shows the evolution of the fluctuation energy $E_<$ and particle number $A_<$ versus the corresponding equilibrium isentropes $S=\mathrm{const}$ for a homogeneous low-amplitude ($|\phi|=0.3$) initial state $E_<=E=2A$ and $A_<=A$. The boundary between $\Delta_<$ and $\Delta_>$ is $r=1$. The particle-nonconserving system produces no persistent peaks. Instead, it increases its entropy by increasing the total number of particles and ends up in a fluctuating high-amplitude state [13]. The particle-conserving system (1) approaches the entropy maximum by generating peaks and transferring energy from the fluctuations $E_<$ to $E_>$. On the other side, growing peaks also absorb particles that must be shifted from $A_<$ to $A_>$. The trace $(E_<,A_<)$ therefore strives down to the left in Fig. 4. This loss of particles in the fluctuations is unfavorable for the production of entropy. The merging of peaks, however, allows the system to store more energy in the peaks while feeding particles from the peaks back into the fluctuations $A_<$ which leads to an additional increase of the entropy.

A state with only one huge peak is not reached experimentally [Fig. 1(b)]. Instead, a number of coherent structures of moderate height [Fig. 2(b)] survive even on very long time scales (10^7 time steps in numerical simulations). In Fig. 4, the trace $(E_<,A_<)$ does not reach the state of maximum entropy at $(E_<=0,\ A_<\approx 370)$, but ends up at in a state with only half that particle content, and still a positive amount of energy. The coherent structures contain a significant amount of particles, and the entropy of the fluctuations is below its maximum. The reason for this is the eventual breakdown of the two entropy-enhancing mechanisms, First, the merging of peaks becomes impossible because peaks above a certain critical height are immobilized by a lattice-pinning effect. For that reason the trace $(E_<,A_<)$ in Fig. 4 does not cross the isentropes S_3,S_2,S_1. Second, the growth of peaks stops when this leads to no further increase of the fluctuation entropy. This happens when the entropy gain due to the energy transfer to the peaks is matched by the entropy loss due to the particle transfer. For this reason, the trace $(E_<,A_<)$ in Fig. 4 does not approach the line $E_<=0$ any further after $\sim 10^5$ time steps.

The mobility of a peak with an amplitude $|\phi_n|=\sqrt{a}$ at a site n depends on the compatibility of the local conservation of its energy $E=a^2/2$ and its particle number $A=a$ during a possible migration to the site $n+1$. Most of the a particles are gathered at these two lattice sites during the migration. The trajectory of such a migration is therefore close to the intersection of the level set of E and A with the constraint of nonvanishing amplitudes at n and $n+1$ only. These paths are given by $\phi_n(\nu)=\sqrt{a}\sqrt{1-\nu}e^{i\psi}$ and $\phi_{n+1}(\nu)=\sqrt{a}\nu e^{i\alpha(\nu)}e^{i\psi}$ with $\cos\alpha=a\sqrt{\nu-\nu^2}/2$. The parameter ν goes from 0 to 1 during the migration as the particles are shifted from n to $n+1$. ψ is a phase factor. The bottleneck of this process is the intermediate storage of $|\phi|^4$ energy in the coupling term $2\,\mathrm{Re}(\phi_n\phi_{n+1}^*)$. The solvability condition $\cos\alpha\leqslant 1$ for all ν requires that $a\leqslant 4$, so that this migrational path only exists for peaks below a maximum amplitude $|\phi_n(\nu=0)|\leqslant 2$. For higher peaks, it is impossible to conserve both particle number and energy at the instant when $|\phi_n|=|\phi_{n+1}|$. These idealized migrational paths deviate from exact solutions of the DNLS which necessarily have nonvanishing amplitudes for adjacent oscillators at $n-1$, $n+2$, etc. Monte Carlo simulations of paths that include small amplitudes for adjacent oscillators (4–20 lattice sites) show that migrations for slightly higher peaks [$|\phi_n(\nu=0)|<2.28$, Fig. 2(b)] are permitted by the conservation laws. Higher peaks first need to decrease by transferring particles to remote lattice sites before they can move. This defocusing process would require a very unlikely decrease of entropy and the local conservation of particles and energy is therefore statistically favorable. Spontaneous collapses of peaks are only possible if this increases the total entropy, which is the case if the fluctuations have small wavelengths and a positive temperature.

Further growth of the peaks requires a flow both of particles and of energy from the fluctuations to the peaks as the number of pinned peaks is fixed on relevant time scales. This is thermodynamically favorable only if the increase of the entropy due to the energy transfer is bigger than the decrease caused by the particle transfer. This process stops when the trace $(E_<,A_<)$ in Fig. 4 approaches an isentrope tangentially as $\partial E_>/\partial A_>|_{K=\mathrm{const}}=\partial E_</\partial A_<|_{S=\mathrm{const}}$ which is equivalent to $\gamma=R^2$. On this line, growth or decay processes of peaks absorb or release energy and particles in a ratio that amounts to isentropic changes of the fluctuations. The statistical results reflect microscopic dynamical findings [12] of the growth and decay processes of localized structures perturbed by one or two incoming waves. Long waves lead to growth, short waves to decay of a peak while the radiated harmonics increase the systems entropy. Experimentally, one still finds irregular oscillations of the peak heights, but no average growth. Interactions of peaks and fluctuations that increase the peaks are matched on average by those interactions that

decrease the peaks. Waves with all wave numbers coexist in the state of equilibrium where growth processes are balanced by decay processes. Any changes of the peak amplitude are statistically unfavorable as they decrease the total entropy.

To conclude, localization in nonintegrable systems constrained by two integrals of motion is a *statistical* process. The entropy is dominated by contributions from small-amplitude fluctuations. The entropy is maximal if an optimal share of each conserved quantity is allocated to the fluctuations. There is no localization if not enough energy is supplied by the initial conditions. If a surplus of energy is provided by the initial conditions, it is dumped into high-amplitude structures that absorb high amounts of energy (Fig. 2) while using few particles. This explains the phase where energy localization occurs. The lattice pinning effect related to the conservation laws prevents the system from reaching the absolute entropy maximum. For the final peak size, growth and decay interactions of the peaks with the fluctuations are balanced.

Obviously, the statistical analysis shows the macroscopic properties of an ensemble of microstates, and one might expect that the Arnold diffusion process transfers the trajectory from any initial condition to this most probable state. However, the thermalization may have extremely long transients. In the numerical simulations, the amplitudes in the initial conditions were small enough so that the separation of the partition function in the statistical description was valid, but large enough for the nonintegrability to have an impact on moderate time scales. In the ''integrable'' limit of smooth initial conditions with very low amplitudes, the dynamics is most similar to the continuous one dimensional nonlinear Schrödinger equation, which is integrable. Consequently, this part of the phase space is partitioned by Kolmogorov-Arnold-Moser tori that are not destroyed by the nonintegrability and the dynamics is quasiperiodic on very long time scales. To escape from this state, the amplitude has to reach a sufficient height so that the nonlinearity absorbs a substantial amount of energy, which becomes a rare event for small average amplitudes. Such quantities that are almost conserved on moderate time scales can also be relevant for localization effects in systems where the Hamiltonian is the only exactly conserved quantity. For instance, the DNLS with broken rotational symmetry shows energy localization on shorter time scales where the particle number changes very little. This is the case in the early stadium of the path $E_<, A_<$ where A is not conserved in Fig. 4. It is an interesting question if this also applies to other breather systems where the Hamiltonian is the only conserved quantity [6,14].

The mechanism of localization is found in very diverse dynamical systems as it relies only on the properties of the entropy functional and on the existence of two conserved quantities and not on the spatial discreteness. Depending on the type of the nonlinearity, the localized structures may absorb primarily the second conserved quantity [8] and not the energy. In continuous systems described by partial differential equations [9,11], the transport of fluctuations is continued down to the molecular scale. Again, the conservation laws require the formation of localized structures for this exploitation of degrees of freedom on short space scales.

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