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Statistical mechanics of the discrete nonlinear Schrödinger equation is studied by means of analytical and numerical techniques. The lower bound of the Hamiltonian permits the construction of standard Gibbsian equilibrium measures for positive temperatures. Beyond the line of $T = \infty$, we identify a phase transition, through a discontinuity in the partition function. The phase transition is demonstrated to manifest itself in the creation of breather-like localized excitations. Interrelation between the statistical mechanics and the nonlinear dynamics of the system is explored numerically in both regimes.

The pioneering studies of Fermi, Pasta and Ulam [1] (FPU) showed that energy exchange between coupled systems may be suppressed in the presence of nonlinearity; instead a type of behavior that severely contrasts equipartition among the linear modes is observed. The question of whether equipartition of excitation energy always appears is a contemporary issue in various fields of physics. Many manifestations of nonequilibrium and non-equipartition phenomena equivalent to the dynamical behavior of systems with few degrees of freedom contrasting statistical mechanics expectations have been observed. Some of these phenomena, and therefore the absence of immediate equipartition expressed in terms of self-trapping of energy, play an important role for optical storage patterns in nonlinear fibers, condensed matter physics, and biophysics [2].

A particularity of discrete nonlinear systems is their ability to sustain strong localization of energy [3]. This is accomplished via *intrinsic localized modes* (*breathers*) which are modes that remain stable for extremely long times. So far it is a largely unaddressed problem how to handle and describe these excitations in a statistical mechanics framework although it has been argued that breathers may act as virtual bottlenecks [4] delaying the thermalization process.

In this work, we develop a statistical understanding of the dynamics, including the breathers, in a discrete nonlinear Schrödinger (DNLS) equation. The DNLS equation plays a significant role in several branches nonlinear physics as a simple physical model because it may approximate many of the above mentioned nonlinear systems. We study analytically and numerically the thermalization of the lattice for $T \geq 0$. We identify the regime in phase space wherein regular statistical mechanics considerations apply, and hence, thermalization is observed numerically and explored analytically using regular, grand-canonical, Gibbsian equilibrium measures. However, the nonlinear dynamics of the problem renders permissible the realization of regimes of phase space which would formally correspond to "negative temperatures" [5] in the sense of statistical mechanics. The novel feature of these states is that the energy tends to be localized in certain lattice sites forming breather-like excitations. Returning to statistical mechanics, such realizations, which would formally correspond to negative temperatures, are not possible (since the Hamiltonian is unbounded from above, as is seen by a simple scaling argument similar to the continuum case [6]) unless one refines the grand-canonical Gibbsian measure to correct for that. This correction will necessitate a discontinuity in the partition function signaling a phase transition that we identify, numerically, with the appearance of breather modes.

In order to explore and illustrate the scenario described above we consider the one-dimensional DNLS equation in the form

$$i\dot{\psi}_m + (\psi_{m+1} + \psi_{m-1}) + \nu|\psi_m|^2\psi_m = 0 \,, \qquad (1)$$

where the overdot denotes time derivative, m is a site index, and ν is a tunable coefficient to the nonlinear term [7]. Equation (1) is the equation of motion, $\dot{\psi}_m = -\frac{\partial \mathcal{H}}{\partial i\psi_m^*}$, where $\mathcal{H}$ is the Hamiltonian function given by

$$\mathcal{H} = \sum_m \left(\psi_m^*\psi_{m+1} + \psi_m\psi_{m+1}^*\right) + \sum_m \frac{\nu}{2}|\psi_m|^4 \,,$$

for which $i\psi_m^*$, ψ_m form canonically conjugate pairs of variables. In addition to the conserved energy $\mathcal{H}$, the quantity $\mathcal{A} = \sum_m |\psi_m|^2$, is also conserved by the dynamics of Eq. (1) and serves as the norm of the system.

In order to study the statistical mechanics of the system, we calculate the classical grand-canonical partition function $\mathcal{Z}$. We first apply the canonical transformation

$\psi_m = \sqrt{A_m}\exp(i\phi_m)$, leading to

$$\mathcal{H} = \sum_m 2\sqrt{A_m A_{m+1}}\cos(\phi_m - \phi_{m+1}) + \frac{\nu}{2}\sum_m A_m^2 \ .$$

The partition function then becomes,

$$\mathcal{Z} = \int_0^\infty \int_0^{2\pi} \prod_m d\phi_m dA_m \exp[-\beta(\mathcal{H} + \mu\mathcal{A})] \ , \qquad (2)$$

where the multiplier μ is introduced in analogy with a chemical potential to ensure conservation of $\mathcal{A}$. Straightforward integration over the phase variable ϕ_m reduces the symmetrized partition function to,

$$\mathcal{Z} = (2\pi)^N \int_0^\infty \prod_m dA_m I_0(2\beta\sqrt{A_m A_{m+1}})\times$$
$$\exp\left[-\beta\sum_m\left(\frac{\nu}{4}(A_m^2 + A_{m+1}^2) + \frac{\mu}{2}(A_m + A_{m+1})\right)\right].$$

This integral can be evaluated exactly in the thermodynamic limit of a large system ($N \to \infty$) using the eigenfunctions and eigenvalues of the transfer integral operator [8],

$$\int_0^\infty dA_m\, \kappa(A_m, A_{m+1})\, y(A_m) = \lambda\, y(A_{m+1}),$$

where the kernel κ is

$$\kappa(x,z) = I_0\left(2\beta\sqrt{xz}\right) \times \exp\left[-\beta\left(\frac{\nu}{4}\left(x^2+z^2\right) + \frac{\mu}{2}(x+z)\right)\right]. \qquad (3)$$

Similar calculations have been performed for the statistical mechanics of the ϕ^4 field [8], and for models of DNA denaturation [9]. One obtains $\mathcal{Z} \simeq (2\pi\lambda_0)^N$, as $N \to \infty$ where λ_0 is the largest eigenvalue of the operator. From this expression the usual thermodynamic quantities such as the free energy, F, or specific heat can be calculated. More importantly, for our purpose we can obtain the averaged energy density, $h = \langle\mathcal{H}\rangle/N$, and the average excitation norm, $a = \langle\mathcal{A}\rangle/N$ as

$$a = -\frac{1}{\beta\lambda_0}\frac{\partial\lambda_0}{\partial\mu}, \quad h = -\frac{1}{\lambda_0}\frac{\partial\lambda_0}{\partial\beta} - \mu a.$$

The average excitation norm a can also be calculated as $a = \frac{1}{\mathcal{Z}}\int_0^\infty \prod_m dA_m\, A_m \exp\left[-\beta\left(\mathcal{H} + \mu\mathcal{A}\right)\right]$, where the integral again can be calculated using the transfer technique [8] and yields $a = \int_0^\infty y_0^2(A) A\, dA$, where y_0 is the normalized eigenfunction corresponding to the largest eigenvalue λ_0 of the kernel κ (Eq. (3)). This shows, that $p(A) = y_0^2(A)$ is the probability distribution function (PDF) for the amplitudes A.

The problem is now reduced to finding the largest eigenvalue λ_0 and the corresponding eigenfunction y_0 of the transfer operator, Eq. (3). This we do numerically. However, two limits ($\beta \to \infty$ and $\beta \to 0$) are also amenable to analytical treatment.

First, notice that the Hamiltonian is bounded from below and one can observe that this minimum is realized by a plane wave, $\psi_m = \sqrt{a}\exp im\pi$, whose energy density is $h = -2a + \frac{\nu}{2}a^2$. This relation defines zero temperature, or the $\beta = \infty$ line.

The high temperature limit is also tractable. When $\beta \ll 1$ the modified Bessel function in the transfer operator can be approximated, to leading order, by unity (this amounts to neglecting the coupling term in the Hamiltonian). This allows us to reduce the remaining eigenvalue problem to the approximate solution valid for thermalized independent units,

$$y_0(A) = \frac{1}{\sqrt{\lambda_0}}\exp\left[-\frac{\beta}{4}\left(\nu A^2 + 2\mu A\right)\right] \ .$$

Using this approximation we can, enforcing the constraint $\beta\mu = \gamma$ (where γ remains finite as we take the limits $\beta \to 0$ and $\mu \to \infty$), obtain $h = \nu/\gamma^2$ and $a = 1/\gamma$. Thus, we get $h = \nu a^2$ at $\beta = 0$.

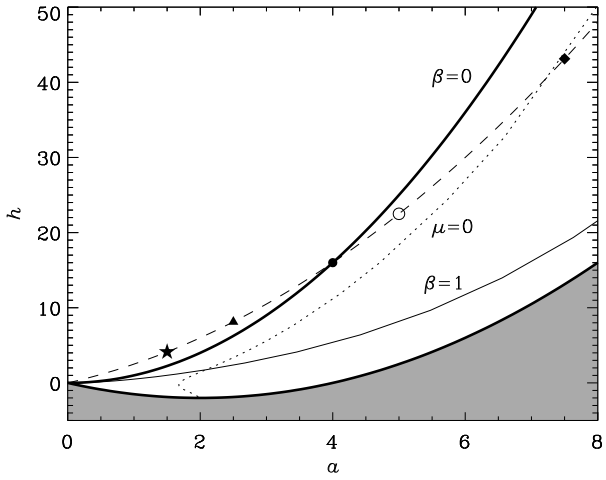

FIG. 1. Parameter space (a, h), where the shaded area is inaccessible. The thick lines represents the $\beta = \infty$ and $\beta = 0$ lines and thus bound the Gibbsian regime. The dashed line represents the $h = 2a + \frac{\nu}{2}a^2$ line along which the reported numerical simulations are performed (pointed by the symbols).

Figure 1, depicts (with thick lines) the two parabolas in (a, h)-space corresponding to the $T = 0$ and $T = \infty$ limits. Within this region all considerations of statistical mechanics in the grand-canonical ensemble are normally applicable and there is a one-to-one correspondence between (a, h) and (β, μ). Thus, within this range of parameter space one expects the system to thermalize in accordance with the Gibbsian formalism. However, the region of the parameter space that is experimentally (numerically) accessible is actually wider since it is possible to initialize the lattice at any energy density h and norm

density a above the $T = 0$ line in an infinite system.

A statistical treatment of the remaining domain of parameter space can be accomplished introducing formally negative temperatures. But the partition function (2) is not suited for that purpose since the constraint expressed in the grand-canonical form fails to bound the Hamiltonian from above. In all the alternative approaches of the study of negative temperatures we will have to consider a finite system of size N. As suggested in [6] we can still consider the grand-canonical ensemble using the modified partition function $\mathcal{Z}'(\beta,\mu') = \int \exp(-\beta(\mathcal{H}+\mu'\mathcal{A}^2)) \prod_m d\psi_m d\psi_m^*$, but this introduces long range coupling and μ' will have to be of order $1/N$. Now β can be negative since $\mathcal{H}+\mu'\mathcal{A}^2$ can be seen to be bounded from above when $\mu' < -\nu/2N$. The important consequence of this explicit modification of the measure, is a jump discontinuity in the partition function, that in turn signals a phase transition. More explicitly, if one starts in a positive T, thermalizable (in the Gibbsian sense) state in phase space with $h > 0$, and continuously varies the norm, then one will, inevitably, encounter the $\beta = 0$ parabola. Hence, in order to proceed in a continuous way, a discontinuity has to be assigned to the chemical potential. This discontinuity will destroy the analyticity of the partition function as the transition line is crossed, and will indicate a phase transformation according to standard statistical mechanics.

From the microcanonical point of view it is also natural to consider negative temperatures because it is possible to maximize the energy under the constraint of fixed norm in a finite system. It can be seen that the configuration which realizes this maximum is an exact breather solution, whose total energy and frequency scale as $\mathcal{A}^2$ and N, respectively. Thus, the number of microstates sharing the same energy E will decrease with increasing E if the norm $\mathcal{A}$ is kept fixed. Due to the definition of temperature ($1/T = \partial S/\partial E|_{\mathcal{A}}$), T becomes negative at high energy density and the $\beta = 0$ line is the line of maximum entropy. Actually we can say that the constraint of fixed norm $\mathcal{A}$ is a "topological" reason for large amplitude breather-like excitations to be expected to appear.

In order to characterize the dynamics of both phases (above and under the $\beta = 0$ line) and to verify that the system does relax to a thermalized state, we perform numerical experiments. We restrict the parameters (a, h) to the dashed-line of Fig. 1, choosing a perturbed phonon with wavevector $q = 0$ ($\psi_m = \sqrt{a}$), for which the energy norm relationship is $h = 2a + \frac{\nu}{2}a^2$ as initial condition. An infinitesimal perturbation to such a linearly unstable mode for systems of oscillators or nonlinearly coupled particles, is well-known [4,10] to give rise to long-lived localized excitations via modulational instabilities. For these initial conditions, the important question is whether the same phenomenology appears in the DNLS system; i.e., whether relaxation to equilibrium is really achieved and whether we can observe different qualitative behavior on the two sides of the $\beta = 0$ line.

Figure 2 shows three typical examples of what can be observed when the energy-norm density point lies below the $\beta = 0$ line (the symbols refer to Fig. 1). The $q = 0$ wave is unstable and the energy density forms small localized excitations but their lifetime is not very long and, rapidly, a stationary distribution of the amplitudes A_m is reached (Fig. 2). Different kinds of initial conditions (with same energy and norm densities) produced the same results. In conclusion, the system reaches an equilibrium state which is perfectly recovered by means of the transfer operator method. Moreover it can be checked on Fig. 2 that the curvature of $\log p(A)$ (i.e., $-\beta$) tends to zero when $h = \nu a^2$. (The cut-off at high amplitudes is due to finite size effects). In this domain of parameter space, high amplitude excitations are highly improbable and can be considered as simple fluctuations; as shown on Fig. 2, large amplitude fluctuations have been recorded but were checked in the evolution pattern to disappear rapidly.

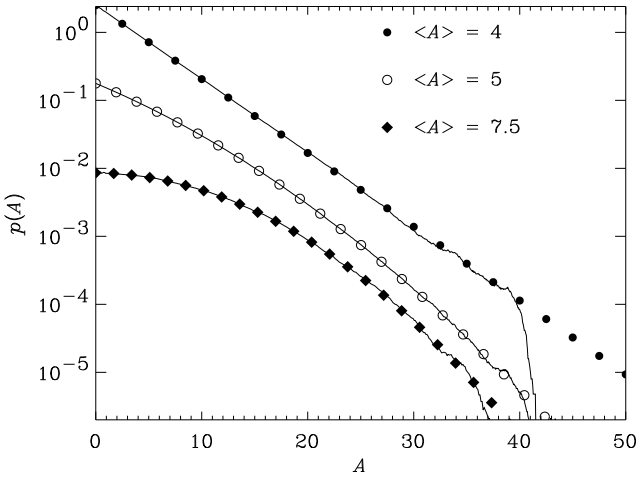

FIG. 2. Distribution of $A = |\psi|^2$ for three cases under (and on) the transition line. The solid lines show the results of simulations and the symbols are given by the transfer operator. Curves are vertically shifted to facilitate visualization.

The scenario is very different when the energy and norm densities are above the $\beta = 0$ line. We can observe a rapid creation of breather excitations due to the modulational instability accompanied by thermalization of the rest of the lattice. Once created, these localized excitations remain mostly pinned and because the internal frequency increases with amplitude their coupling with the small amplitude radiation is very small. This introduces a new time scale in the thermalization process necessitating simplectic integration for as long as $10^6 - 10^7$ time units in order to reach a stationary PDF. This can also be qualitatively justified by the effective long range interactions, introduced in the modified partition function, which will produce stronger memory effects as one

observes regimes in phase space which are further away from the transition line (since the long range interaction will be stronger).

Typical distribution functions of the amplitudes are shown in Fig. 3. The presence of high amplitude excitations is directly seen here (more straightforwardly we observed standing breathers in the spatial pattern). The dotted line represents the PDF in the case where the initial condition is chosen at random, using a larger system size: we check that the initial condition seems unimportant, but the system size does influence the amplitude of the highest breathers. The cut-off value in the very large system limit, as well as the persistence of a bump in the PDF, is still an open question, since we have no prediction for the PDF above the $\beta = 0$ line. However the positive curvature of the PDF at small amplitudes clearly indicates that the system evolves in a regime of negative temperature and the appearance of the phase transformation is signified in the dynamics by the appearance of these strongly localized persistent breathers.

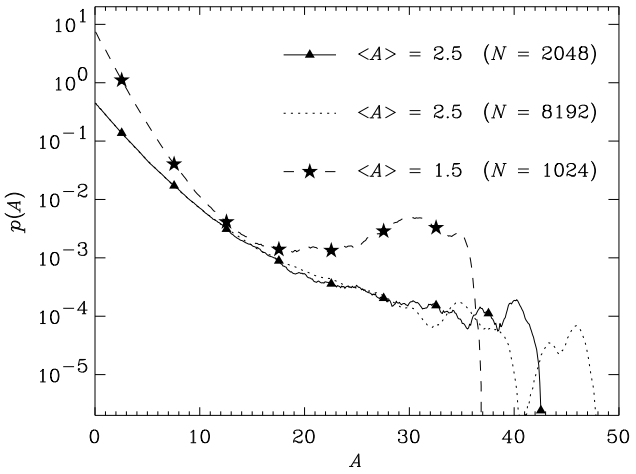

FIG. 3. Distribution of $A = |\psi|^2$ for parameters (h, a) above the transition line (triangles and stars as in Fig. 1).

The actual dynamics in the negative temperature regime is studied more closely in Ref. [11].

Finally, we can draw an interesting parallel with what has been known in plasma physics and hydrodynamics for several years [12], where the appearance of localized structures (of vortices in that case) is also related to a description in terms of negative temperatures.

In conclusion, studying the DNLS system, we have been able to quantify and explain, through analytical calculations supported by numerical computations, the behavior in different regimes of the (h, a) phase space. We have been able to link the regime of thermalization to the regime where regular statistical mechanics is applicable in the Gibbsian sense. Further, we have traced the explanation of the appearance of localized modes in different regimes in phase space to the need for a modified measure to ensure normalizability, which therefore necessitates a phase transition leading to these localized modes. Our numerical simulations strongly support this theoretical picture, illuminating this novel quantitative connection between nonlinear dynamics and statistical mechanics.

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