

Equilibrium and nonequilibrium description of negative temperature states in a one dimensional lattice using a wave kinetic approach

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We predict negative temperature states in the Discrete Nonlinear Schrödinger (DNLS) equation as exact solutions of the associated Wave Kinetic equation. Within the wave kinetic approach, we define an entropy that results monotonic in time and reaches a stationary state, that is consistent with classical equilibrium statistical mechanics. We also perform a detailed analysis of the fluctuations of the actions at fixed wave numbers around their mean values. We give evidence that such fluctuations relax to their equilibrium behaviour on a shorter time scale than the one needed for the spectrum to reach the equilibrium state. Numerical simulations of the DNLS equation are shown to be in agreement with our theoretical results. The key ingredient for observing negative temperatures in lattices characterized by two invariants is the boundedness of the dispersion relation.

INTRODUCTION

Negative temperatures have been the subject of intensive studies since they were conceived in the study of point vortices [1] and the subsequent experimental work in [2], where negative temperatures in nuclear spin systems were observed. More recently, negative temperatures were also observed in ultra-cold quantum systems [3]; moreover, the predictions of Onsager on point vortices have been verified experimentally [4, 5]. In thermodynamics the requirement for observing negative temperatures is that the entropy S does not increase monotonically with energy. Indeed, if the entropy is a continuous function of the energy, E , reaching a maximum away from its domain boundary, negative temperatures are expected. This descends from the thermodynamic definition of temperature, $T = (\partial S / \partial E)^{-1}$. As expressed in [6], “the assumption of monotonic increase of the entropy with the energy is not essential to the development of thermodynamics...”. Despite controversies and criticisms to the existence of negative temperatures related to the definition of the entropy [7, 8], negative temperatures are now well accepted by a vast community and the observations in experiments appear to be reliable [9–14].

Here, we present an approach to the theory of negative temperatures in weakly anharmonic lattices based on the so called Wave Kinetic (WK) equation [15, 16], i.e. an equation that, in analogy with the Boltzmann equation for particles, describes the mesoscale dynamics of a system of interacting waves. The WK equation can be derived in a systematic way from deterministic (microscopic) weakly nonlinear and dispersive wave systems [15–17]. It has been applied to a variety of fields such as nonlinear optics [18], surface gravity waves [19, 20], Bose-Einstein condensation [21, 22], gravitational waves [23], vibrations in anharmonic lattices [24, 25]. In this Re-

port, we will consider the Discrete Nonlinear Schrödinger (DNLS) equation as the starting point, and build its thermodynamic properties in the limit of small nonlinearity, passing through a mesoscopic description via the WK equation.

The DNLS equation, [26], as its continuous version, is a universal model; it describes the propagation of optical waves in a waveguide array or a Bose-Einstein condensate in a periodic optical lattice. Differently from other discrete systems, like the Fermi-Pasta-Ulam-Tsingou (FPUT) lattice [27], the DNLS equation has two conserved quantities, i.e the Hamiltonian and the total number of particles (two conservation laws are a fundamental ingredient for observing negative temperatures). A number of previous studies [28–34] have discussed the statistical mechanics of the DNLS equation. The main idea in [28] is that the negative temperatures in DNLS are associated with the emergence of high amplitude localized structures or discrete breathers [35] in the strongly nonlinear regime. Developments using the microcanonical ensemble can be found in [36]. In the field of nonlinear optics some interesting work has been done at equilibrium for a finite number of modes, see [37–40]. Our approach, being based on a theory that makes use of the random phase approximation both for positive and negative temperatures, cannot be applied in the presence of coherent structures such as solitons or breathers. Negative temperatures will reveal themselves as localized Fourier energy spectrum in the high wave number region.

THE WAVE KINETIC THEORY FOR THE DNLS EQUATION

The DNLS equation reads

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

where ψ_n is the complex amplitude of the oscillator at site m , with $m = 1, 2, \dots, M$ and ν is an anharmonic parameter that weighs the nonlinearity of the system. The DNLS equation has two conserved quantities:

$$\begin{aligned} H &= \sum_{m=1}^M \left(|\psi_{m+1} - \psi_m|^2 - \frac{1}{2}\nu |\psi_m|^4 \right), \\ N &= \sum_{m=1}^M |\psi_m|^2. \end{aligned} \quad (2)$$

which are the Hamiltonian and the total conserved norm of the DNLS equation, respectively.

In our work we will use periodic boundary conditions and, using the following convention for the Discrete Fourier Transforms,

$$\psi_m = \sum_{k=1}^M \hat{\psi}_k e^{i2\pi km/M}, \quad \hat{\psi}_k = \frac{1}{M} \sum_{n=1}^M \psi_n e^{-i2\pi kn/M}, \quad (3)$$

we write the equation in Fourier space as

$$i\dot{\hat{\psi}}_{k_1} = \omega_{k_1} \hat{\psi}_{k_1} - \nu \sum_{k_2, k_3, k_4} \hat{\psi}_{k_2}^* \hat{\psi}_{k_3} \hat{\psi}_{k_4} \delta_{12}^{34}, \quad (4)$$

where $\omega_k = 4 \sin^2(\pi k/M)$ and $\delta_{12}^{34} = \delta_{k_1+k_2, k_3+k_4}$ is the Kronecker δ that accounts for Umklap processes, i.e. $k_1 + k_2 = k_3 + k_4 \pmod{M}$. The Hamiltonian in Fourier space takes the following form:

$$\frac{H}{M} = \sum_{k_1} \omega_{k_1} |\hat{\psi}_{k_1}|^2 - \frac{1}{2}\nu \sum_{k_1 k_2, k_3, k_4} \hat{\psi}_{k_1}^* \hat{\psi}_{k_2}^* \hat{\psi}_{k_3} \hat{\psi}_{k_4} \delta_{12}^{34}, \quad (5)$$

By using the following transformation $\hat{\psi}_k = \sqrt{I_k} \exp(-i\theta_k)$, the equation can be written in angle-action variables:

$$\begin{aligned} \frac{dI_{k_1}}{dt} &= -2\nu \sum \sqrt{I_{k_1} I_{k_2} I_{k_3} I_{k_4}} \sin(\Delta\theta_{12}^{34}) \delta_{12}^{34}, \\ \frac{d\theta_{k_1}}{dt} &= \omega_{k_1} - \nu \sum \sqrt{\frac{I_{k_2} I_{k_3} I_{k_4}}{I_{k_1}}} \cos(\Delta\theta_{12}^{34}) \delta_{12}^{34}, \end{aligned} \quad (6)$$

with $\Delta\theta_{12}^{34} := \theta_{k_1} + \theta_{k_2} - \theta_{k_3} - \theta_{k_4}$. Assuming that $\nu \ll 1$, we expand the action-angle variables in powers of ν ; we then assume that the initial angles (or phases) are independent random variables uniformly distributed in the $[0, 2\pi)$ interval. A key step consists in taking the large box limit, which implies taking $M \rightarrow \infty$, thus making the Fourier modes dense in the interval $[0, 2\pi)$. The Wave Kinetic equation (Boltzmann equation for phonons) can then be obtained (see [17] for details on the derivation):

$$\frac{dn_{k_1}}{d\tau} = \xi_{k_1} - \gamma_{k_1} n_{k_1} \quad (7)$$

with

$$\begin{aligned} \xi_{k_1} &= 4\pi\nu^2 \int_0^{2\pi} n_{k_2} n_{k_3} n_{k_4} \delta(\Delta\omega_{12}^{34}) \delta_{12}^{34} dk_{234} \\ \gamma_{k_1} &= -4\pi\nu^2 \int_0^{2\pi} (n_{k_3} n_{k_4} - n_{k_2} n_{k_3} - n_{k_2} n_{k_4}) \times \\ &\delta(\Delta\omega_{12}^{34}) \delta_{12}^{34} dk_{234}, \end{aligned} \quad (8)$$

where $\Delta\omega_{12}^{34} = \omega_{k_1} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4}$, k is a continuous variable in the $[0, 2\pi]$ interval, $dk_{234} = dk_2 dk_3 dk_4$, $\omega_k = 4 \sin^2(k/2)$, $n_k = n(k, t) = \langle I_k \rangle M/2\pi$ is the wave action spectral density, and $\langle \cdot \rangle$ is performed over the initial random phases and independent actions. Strictly speaking, the WK equation is valid under the assumption that random phases and amplitudes persist over time [41]. Besides the evolution equation for the spectral density function, using the same approximations and tools, it is also possible to derive an evolution equation for the second moment, $\Lambda_k = \langle I_k^2 \rangle (M/2\pi)^2$, which reads:

$$\frac{d\Lambda_{k_1}}{d\tau} = 4n_{k_1} \xi_{k_1} - 2\gamma_{k_1} \Lambda_{k_1}. \quad (9)$$

Such an equation, see [15, 42], describes the fluctuations of the wave action density at fixed wave number. The solution of the Cauchy problem for the coupled system (7-9) requires numerical computations; however, some interesting physical insights can be achieved by making the following analysis.

The WK equation for phonons has two invariants:

$$E = \int_0^{2\pi} \omega(k) n(k, t) dk, \quad N = \int_0^{2\pi} n(k, t) dk, \quad (10)$$

which are named energy and number of particles or wave action (strictly speaking, energy and number densities). Here, we point out that the conserved quantities of the WK equation have a counterpart in the DNLS equation; however, there is a major difference: while the number of particles is conserved in both models, the energy conserved by the WK equation corresponds to the harmonic part of the Hamiltonian, see eq. (5), appropriately averaged. By defining the entropy density (see [16, 43]), as:

$$S(t) = \int_0^{2\pi} \ln n(k, t) dk, \quad (11)$$

an H theorem, $dS/dt \geq 0$, holds. When, and only when $dS/dt = 0$, the Rayleigh-Jeans (RJ) distribution is obtained:

$$n(k)^{(RJ)} = \frac{T}{\omega(k) - \mu} = \frac{1}{\beta\omega(k) - \gamma}. \quad (12)$$

Here T and μ are usually named temperature and chemical potential ($\beta = 1/T$ and $\gamma = \mu/T$). This result is consistent with classical equilibrium statistical mechanics, see [10], eq. (58) therein). Because $n(k)$ is positive

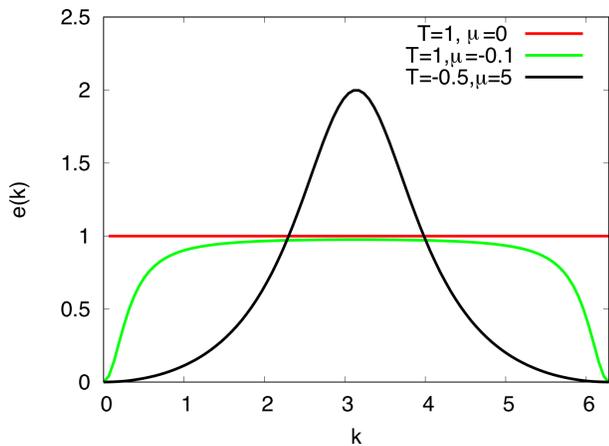


FIG. 1. Spectral energy density $e(k) = \omega(k)n(k)$ for different temperatures and chemical potentials. The red horizontal line is the typical equipartition of energy and corresponds to $T = 1$ and $\mu = 0$; the green line corresponds to $T = 1$ and $\mu = 0.1$ and the light blue line (sharply peaked around $k = \pi$) corresponds to negative temperatures, i.e. $T = -0.5$ and $\mu = 5$. All these curves are exact stationary solutions of the WK equation.

for all k , at equilibrium one of the following conditions holds:

$$\begin{aligned} \beta > 0 \quad \text{and} \quad \gamma < 0, \quad \text{or} \\ \beta < 0 \quad \text{and} \quad \gamma < 4\beta. \end{aligned} \quad (13)$$

As noted in [10], the last condition implies the existence of negative temperatures. In Figure 1 we show the spectral energy density, $e(k) = \omega(k)n(k)$, as a function of k for different temperatures and chemical potentials. The classical equipartition of energy, typical of systems that conserve only energy, is obtained by setting $\mu = 0$. In Figure 1, a stationary state with $T < 0$ and $\mu > 0$ is also displayed. All of the states represented in Figure 1 are stationary states of the WK equation.

Negative temperatures are characterized by a peaked distribution around $k = \pi$.

Besides mean values, the wave kinetic approach offers the possibility to investigate the fluctuations and their relaxation time scale. It can be checked by substitution that a non stationary solution of equation (9) is $\Lambda_k(t) = 2n_k^2(t)$, provided $n_k(t)$ evolves according to (7). The understanding of the time scale by which such solution is approached is extremely interesting. Because of their similar mathematical structure, one may expect that equations (7) and (9) evolve on the same time scale. As a matter of fact, it will be shown in the numerical computations that $\Lambda_k(t)$ approaches $2n_k^2(t)$ on a much faster time scale than the one pertaining to the evolution of n_k . Indeed, assuming that $\Lambda_k(t)$ is characterized by two time scales, the longer one being the same as the one for $n_k(t)$, it is straightforward to show from eq. (9)

that $\Lambda_k(t)$ reaches $2n_k(t)^2$ exponentially fast and then it remains enslaved to it, as it tends to its asymptotic value.

Equilibrium and thermodynamics

It is not obvious a priori to what extent the variables used in the WK equation correspond to the ones appearing in the first law of thermodynamics. Here, we show that they satisfy the equilibrium classical relation between T and S , i.e. $T = (\partial S / \partial E)^{-1}$. Given the energy, E , the number of particles, N , and S at equilibrium, i.e. for $n(k, t) = n(k)^{(R,J)}$, we obtain (similar integrals were calculated in [33] to study the erosion of a discrete breather by a thermal bath):

$$\begin{aligned} E(\gamma, \beta) &= \frac{2\pi}{\beta} \left(1 + \frac{\gamma}{\sqrt{\gamma(\gamma - 4\beta)}} \right), \\ N(\gamma, \beta) &= \frac{2\pi}{\sqrt{\gamma(\gamma - 4\beta)}}, \end{aligned} \quad (14)$$

$$S(\gamma, \beta) = 2\pi \ln \left[\frac{2}{2\beta - \gamma + \sqrt{\gamma(\gamma - 4\beta)}} \right]. \quad (15)$$

To express the entropy as a function of energy and number of particles, $S(E, N)$, we invert the relations in (14):

$$\beta(E, N) = \frac{4\pi(E - 2N)}{E(E - 4N)}, \quad \gamma(E, N) = \frac{2\pi E}{N(E - 4N)}. \quad (16)$$

Knowing that $\gamma = \mu/T$, the expression for the chemical potential can be derived:

$$\mu(E, N) = \frac{E^2}{2(E - 2N)N}. \quad (17)$$

A phase diagram with the energy as a function of number of particles for fixed temperature can be easily built by solving the first of equations (16) for the energy to obtain:

$$E = 2N + 2\pi T - 2\text{sgn}[T] \sqrt{N^2 + \pi^2 T^2}. \quad (18)$$

For $T \rightarrow 0^+$, we have $E \rightarrow 0$; for $T \rightarrow 0^-$, we have $E \rightarrow 4N$ from below; for $T \rightarrow \pm\infty$, we get $E \rightarrow 2N$.

Interestingly, since γ is always negative, there is an upper value for the energy for fixed number of particles, i.e. $0 < E < 4N$. Moreover, a positive β requires $E < 2N$. Then, negative values of β , i.e. negative temperatures, are possible only for $2N < E < 4N$. For positive temperatures, the chemical potential is negative and becomes positive for negative temperatures, with the constrain that $\mu > 4$. These results are shown in Figure 2. Plugging equations (16) into (15), we obtain:

$$S(E, N) = 2\pi \ln \left[\frac{E(4N - E)}{8\pi N} \right], \quad (19)$$

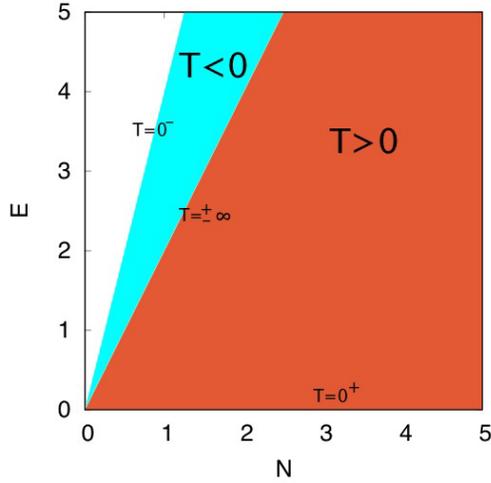


FIG. 2. Energy, E , as a function of the number of particles, N . The white region corresponds to non accessible energies, the light blue to negative temperatures and the red to positive temperatures. The lines corresponding to 0^+ , 0^- and $\pm\infty$ temperatures are also visible. $T = 0^-$ corresponds to $E = 4N$, $T = \pm\infty$ to $E = 2N$ and $T = 0^+$ to $E = 0$

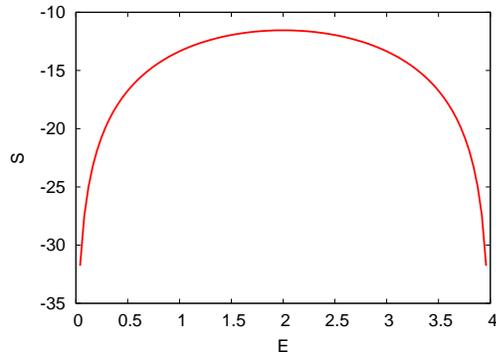


FIG. 3. The entropy, S , as a function of the energy, E , for $N = 1$. The derivative of S is the inverse of the temperature. For $E > 2N=2$ the derivative is negative, implying a negative temperature. Note that entropy is defined for $0 < E < 4N$

see also [30]. The entropy is defined for $0 < E < 4N$; it is a continuous function of its arguments and it has an absolute maximum at $E = 2N$. For fixed E and large N , there is a horizontal asymptote at $N = 2\pi \ln[E/(2\pi)]$ which corresponds to $\gamma = 0$. In Figure (3), we show the entropy as a function of the energy E for $N = 1$.

The above description is consistent with the formalism of classical thermodynamics; indeed, differentiating the entropy

$$dS(E, N) = \left(\frac{\partial S}{\partial E}\right)_N dE + \left(\frac{\partial S}{\partial N}\right)_E dN \quad (20)$$

and calculating the derivatives, it turns out that $(\partial S/\partial E)_N = \beta$ and $(\partial S/\partial N)_E = -\gamma$. This implies that the definition of entropy and other variables in the

WK equation at the Rayleigh-Jeans equilibrium match the corresponding definitions given in classical thermodynamics.

The Boltzmann entropy and its relation to the nonequilibrium entropy defined in equation (11)

The Boltzmann entropy S_B is proportional to the natural logarithm of the number of possible microstates Ω of a system at fixed energy and number of particles:

$$S_B = \ln \Omega. \quad (21)$$

The strategy to compute Ω is the following: we consider $\Omega(N, H)$ and take a two-dimensional Laplace transform to get $\Omega(\gamma, \beta)$:

$$\Omega(\gamma, \beta) = \int_0^\infty \Omega(N, H) e^{\gamma N - \beta H} dH dN \quad (22)$$

$\Omega(N, H)$ can be calculated as

$$\Omega(N, E) = \int_0^\infty \delta\left(N - \sum_{k=1}^M I_k\right) \delta\left(E - \sum_{k=1}^M \omega_k I_k\right) \prod_{k=1}^M dI_k, \quad (23)$$

where, consistently with our hypothesis related to the random phases and the smallness of the nonlinearity, we have assumed $H \simeq E$, with E the harmonic energy density. We plug (23) in (22) and use the property of the δ , so that

$$\Omega(\gamma, \beta) = \int_0^\infty e^{\gamma \sum_{k=1}^M I_k - \beta \sum_{k=1}^M \omega_k I_k} \prod_{k=1}^M dI_k, \quad (24)$$

which can be rewritten as:

$$\Omega(\gamma, \beta) = \int_0^\infty \prod_{k=1}^M e^{\gamma I_k - \beta \omega_k I_k} dI_k. \quad (25)$$

The dependence on I_k has been factorized and we can integrate over I_k to get

$$\Omega(\gamma, \beta) = \prod_{k=1}^M \frac{1}{-\gamma + \beta \omega_k}. \quad (26)$$

We then play the usual trick of taking the exponential of a log

$$\Omega(\gamma, \beta) = \exp \left[\ln \prod_{k=1}^M \frac{1}{-\gamma + \beta \omega_k} \right] = \exp \left[\sum_{k=1}^M \ln \frac{1}{-\gamma + \beta \omega_k} \right] \quad (27)$$

Now, we take the large box limit $M = 2\pi/\Delta k \rightarrow \infty$ and using the definition of the Boltzmann's entropy $S_B = \ln \Omega$ we get:

$$S_B(\gamma, \beta) = \ln \Omega(\gamma, \beta) = \frac{M}{2\pi} \int_0^{2\pi} \ln \left[\frac{1}{-\gamma + \beta \omega_k} \right] dk \quad (28)$$

This formula, apart from the factor $M/2\pi$, is our entropy, see equation (11) where $n(k)$ has been taken at equilibrium.

DIRECT NUMERICAL SIMULATIONS OF THE DNLS EQUATION.

The fact that the WK equation predicts the existence of negative temperatures does not necessarily imply that the DNLS equation at small nonlinearity displays stationary solutions with $T < 0$, as the WK equation is formally derived only in the limit of random phases and random amplitudes. A direct numerical simulation of the deterministic equation of motion is needed in order to establish whether the stationary solutions of equations (7) and (9) are compatible with the microscopic dynamics.

The DNLS equation has been solved numerically using a standard 4th-order Runge-Kutta method; the simulations performed preserved the Hamiltonian and the number of particles up to four significant digits. The initial conditions are provided in Fourier space; the complex amplitudes in physical space are recovered using the Discrete Fourier Transform

$$\psi_m = \sum_{k=1}^M \sqrt{n_k \Delta k} e^{i(2\pi km/M)} e^{i\phi_k}, \quad (29)$$

where $\Delta k = 2\pi/M$ and ϕ_k are random phases distributed uniformly in the $[0, 2\pi)$ interval. In order to observe negative temperature, we consider the following Gaussian shaped initial wave action spectral density function:

$$n_k = B + A \exp \left[\frac{-((k - k_0)\Delta k)^2}{(2\sigma^2)} \right] \quad (30)$$

with $\sigma = 0.9$, $A = 2$, $B = 0$, $\Delta k = 2\pi/M$, $M = 512$, $k_0 = M/2$. With this choice $E = \sum \omega_k n_k \Delta k = 18.80$ and $N = \sum n_k \Delta k = 5.63$; therefore $2N < E < 4N$ which corresponds to $T = -0.74$ and $\mu = 4.16$, i.e. negative temperatures. 1000 realizations of the same spectrum (deterministic amplitudes) with different random phases have been considered and the results are obtained by averaging over the ensemble. The nonlinear parameter ν was set to 0.03. In Figure 4 we report the spectral energy density at time $t = 0$, $t = 10^3$ and $t = 10^4$; the RJ prediction with the temperature and chemical potential obtained from theory is also shown; the curves are almost indistinguishable, i.e. the long time behaviour of $e(k)$ matches the theoretical RJ predictions. The simulation was carried out up to time $t = 10^5$ and no further changes in the energy density spectrum were observed (similar results have been obtained in [29]). Moreover, we show in the inset of the figure the monotonicity of the entropy S , as predicted by the H -theorem for the wave kinetic equation, see (11). Similar plots can be obtained

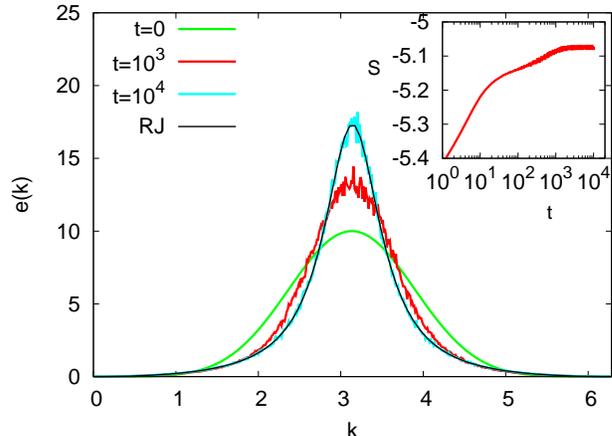


FIG. 4. Energy density as a function of wave number for a simulation of the DNLS equation characterized by the initial condition in (30) that corresponds to $T = -0.74$ and $\mu = 4.16$. Note that, because of the conservation of energy and number of particles, temperature and chemical potential do not change in time [44, 45]. The energy spectral density is the result of averaging over 1000 realizations characterized by different random phases. At the center of the domain, from bottom to top, the curves refer to $t = 0$, $t = 10^3$, $t = 10^4$, respectively, and the dark curve is the prediction from the Rayleigh-Jeans distribution, equation (12). In the inset the entropy defined in eq. (11) as a function of time is displayed.

for positive temperatures. Concerning the fluctuations described by the second moment, we show in Figure 5 the evolution in time of Λ_k for $k = \pi$. The numerical results show that the prediction of equation (9) is accurate: after a very quick relaxation to the solution (shown in the inset), Λ_k follows the evolution $2n_k^2$. The probability density function of I_k is also reported in Figure 6 for different times. The prediction based on the wave kinetic approach is the exponential distribution [15, 41, 46]; the figure shows that the distribution tends very rapidly, on a shorter time scale than the one required for the spectrum to reach its stationary value, to the exponential curve.

DISCUSSION AND CONCLUSIONS

The notion of negative temperatures is well established through some experimental results and theoretical arguments and it is well known that it is strictly connected with the existence of an upper bound for the energy. In our work we have studied negative temperatures in a lattice starting from a microscopic dynamics. The family of stationary equilibrium solutions of the WK equation associated with the lattice dynamics are characterized by two parameters which play the role of temperature and chemical potential. For most of the systems in this framework the temperature is positive and the chemical potential is negative. However, if the dispersion rela-

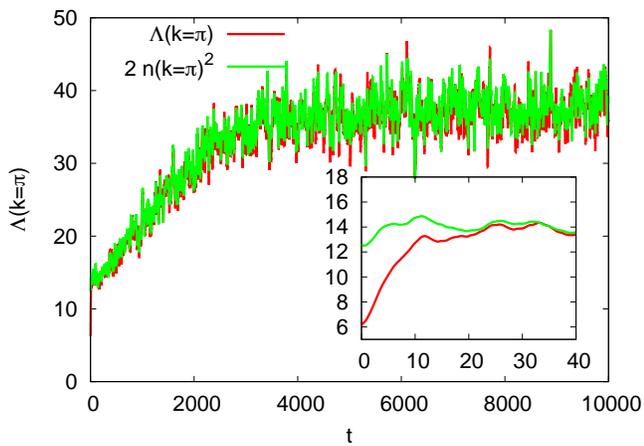


FIG. 5. Evolution in time of the second moment $\Lambda(k = \pi, t)$ in light green. The solution of the equation (9) $\Lambda(k = \pi, t) = 2n(k = \pi, t)^2$ is shown in red. In the inset a zoom of the the early stages of the evolution are also reported.

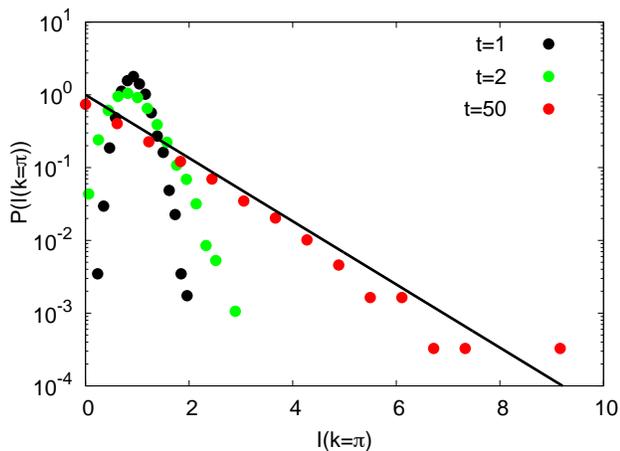


FIG. 6. Probability density function of $I(k = \pi)$ for different times. The dark line corresponds to the exponential distribution derived in Refs.[15, 41, 46]

tion is bounded from above, as in the case of the DNLS equation, then the distribution of particles in wave numbers can be positive also for negative temperatures and positive chemical potential. This simple observation has allowed us to carry out the calculation and express analytically T and μ as functions of the energy and number of particles. Numerical simulations of the lattice dynamics agree well with the theory. Moreover, we have also studied the evolution of the fluctuations around the mean values, i.e. the wave action spectrum; in the framework of the wave kinetic approach it is also possible to derive an equation for the second moment, $\Lambda_k(t)$, of the probability density function of the action; it is interesting to notice that the time scale needed for $\Lambda_k(t)$ to approach its solution, $2n_k^2(t)$, is much faster than the time needed for $n_k(t)$ to reach the Rayleigh-Jeans distribution. The

probability density function of the action is shown to approach the exponential distribution on the fast time scale.

Our analytical result is valid only in the limit of weak nonlinearity, where the unperturbed energy (the one associated with the linear part of the equation of motion) is a quasi-conserved quantity (besides the number of particles). In the presence of a single conservation law, negative temperatures are not predicted because the Rayleigh-Jeans distribution corresponds to the standard equipartition of energy (no chemical potential is present) and temperature may not assume negative values. We also emphasise that our approach, compatible with negative temperatures, is universal and can be applied to many other dispersive wave systems characterized by resonant four-wave interactions, provided the dispersion relation is limited from above, or the Fourier domain is truncated as in the case of inviscid two dimensional turbulence, described in [47]. Indeed, recently, relaxation to a RJ distribution in a multimode optical fiber has been observed [48]; such system is a good candidate for observing experimentally negative temperature.

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- [1] L. Onsager, Statistical hydrodynamics, *Il Nuovo Cimento* (1943-1954) **6**, 279 (1949).
 - [2] E. M. Purcell and R. V. Pound, A nuclear spin system at negative temperature, *Physical Review* **81**, 279 (1951).
 - [3] S. Braun, J. P. Ronzheimer, M. Schreiber, S. S. Hodgman, T. Rom, I. Bloch, and U. Schneider, Negative absolute temperature for motional degrees of freedom, *Science* **339**, 52 (2013).
 - [4] S. P. Johnstone, A. J. Groszek, P. T. Starkey, C. J. Billington, T. P. Simula, and K. Helmerson, Evolution of large-scale flow from turbulence in a two-dimensional superfluid, *Science* **364**, 1267 (2019).
 - [5] G. Gauthier, M. T. Reeves, X. Yu, A. S. Bradley, M. A. Baker, T. A. Bell, H. Rubinsztein-Dunlop, M. J. Davis, and T. W. Neely, Giant vortex clusters in a two-dimensional quantum fluid, *Science* **364**, 1264 (2019).
 - [6] N. F. Ramsey, Thermodynamics and statistical mechanics at negative absolute temperatures, *Physical Review* **103**, 20 (1956).
 - [7] J. Dunkel and S. Hilbert, Consistent thermostatics forbids negative absolute temperatures, *Nature Physics* **10**,

- 67 (2014).
- [8] S. Calabrese and A. Porporato, Origin of negative temperatures in systems interacting with external fields, *Physics Letters A* **383**, 2153 (2019).
- [9] D. Frenkel and P. B. Warren, Gibbs, boltzmann, and negative temperatures, *American Journal of Physics* **83**, 163 (2015).
- [10] P. Buonsante, R. Franzosi, and A. Smerzi, On the dispute between boltzmann and gibbs entropy, *Annals of Physics* **375**, 414 (2016).
- [11] A. Puglisi, A. Sarracino, and A. Vulpiani, Temperature in and out of equilibrium: A review of concepts, tools and attempts, *Physics Reports* **709**, 1 (2017).
- [12] L. Cerino, A. Puglisi, and A. Vulpiani, A consistent description of fluctuations requires negative temperatures, *Journal of Statistical Mechanics: Theory and Experiment* **2015**, P12002 (2015).
- [13] E. Abraham and O. Penrose, Physics of negative absolute temperatures, *Physical Review E* **95**, 012125 (2017).
- [14] M. Baldovin, S. Iubini, R. Livi, and A. Vulpiani, Statistical mechanics of systems with negative temperature, *Physics Reports* (2021).
- [15] S. Nazarenko, *Wave turbulence*, Vol. 825 (Springer Science & Business Media, 2011).
- [16] V. E. Zakharov, V. S. L'vov, and G. Falkovich, *Kolmogorov spectra of turbulence I: Wave turbulence* (Springer Science & Business Media, 2012).
- [17] M. Onorato and G. Dematteis, A straightforward derivation of the four-wave kinetic equation in action-angle variables, *Journal of Physics Communications* (2020).
- [18] A. Picozzi, J. Garnier, T. Hansson, P. Suret, S. Randoux, G. Millot, and D. N. Christodoulides, Optical wave turbulence: Towards a unified nonequilibrium thermodynamic formulation of statistical nonlinear optics, *Physics Reports* **542**, 1 (2014).
- [19] V. E. Zakharov and N. Filonenko, Energy spectrum for stochastic oscillations of the surface of a liquid, in *Doklady Akademii Nauk*, Vol. 170 (Russian Academy of Sciences, 1966) pp. 1292–1295.
- [20] K. Hasselmann, On the non-linear energy transfer in a gravity-wave spectrum part 1. general theory, *Journal of Fluid Mechanics* **12**, 481 (1962).
- [21] S. Nazarenko and M. Onorato, Wave turbulence and vortices in bose–einstein condensation, *Physica D: Nonlinear Phenomena* **219**, 1 (2006).
- [22] D. Proment, S. Nazarenko, and M. Onorato, Quantum turbulence cascades in the gross-pitaevskii model, *Physical Review A* **80**, 051603 (2009).
- [23] S. Galtier and S. V. Nazarenko, Turbulence of weak gravitational waves in the early universe, *Physical Review Letters* **119**, 221101 (2017).
- [24] J. Lukkarinen and H. Spohn, Anomalous energy transport in the fpu- β chain, *Communications on Pure and Applied Mathematics: A Journal Issued by the Courant Institute of Mathematical Sciences* **61**, 1753 (2008).
- [25] M. Onorato, L. Vozella, D. Proment, and Y. V. Lvov, Route to thermalization in the α -fermi–pasta–ulam system, *Proceedings of the National Academy of Sciences* **112**, 4208 (2015).
- [26] P. G. Kevrekidis, *The discrete nonlinear Schrödinger equation: mathematical analysis, numerical computations and physical perspectives*, Vol. 232 (Springer Science & Business Media, 2009).
- [27] E. Fermi, J. Pasta, and S. Ulam, Los Alamos Report LA-1940, E. Fermi, *Collected Papers* **2**, 977 (1955).
- [28] K. Rasmussen, T. Cretegny, P. G. Kevrekidis, and N. Grønbech-Jensen, Statistical mechanics of a discrete nonlinear system, *Physical review letters* **84**, 3740 (2000).
- [29] B. Rumpf, Transition behavior of the discrete nonlinear schrödinger equation, *Physical Review E* **77**, 036606 (2008).
- [30] B. Rumpf, Stable and metastable states and the formation and destruction of breathers in the discrete nonlinear schrödinger equation, *Physica D: Nonlinear Phenomena* **238**, 2067 (2009).
- [31] S. Iubini, S. Lepri, and A. Politi, Nonequilibrium discrete nonlinear schrödinger equation, *Physical Review E* **86**, 011108 (2012).
- [32] S. Iubini, R. Franzosi, R. Livi, G.-L. Oppo, and A. Politi, Discrete breathers and negative-temperature states, *New Journal of Physics* **15**, 023032 (2013).
- [33] B. Rumpf, Growth and erosion of a discrete breather interacting with rayleigh-jeans distributed phonons, *EPL (Europhysics Letters)* **78**, 26001 (2007).
- [34] B. Rumpf, Simple statistical explanation for the localization of energy in nonlinear lattices with two conserved quantities, *Physical Review E* **69**, 016618 (2004).
- [35] S. Flach and C. R. Willis, Discrete breathers, *Physics Reports* **295**, 181 (1998).
- [36] G. Gradenigo, S. Iubini, R. Livi, and S. N. Majumdar, Localization in the discrete non-linear schrödinger equation: mechanism of a first-order transition in the microcanonical ensemble (2019), arXiv:1910.07461 [cond-mat.stat-mech].
- [37] M. Parto, F. O. Wu, P. S. Jung, K. Makris, and D. N. Christodoulides, Thermodynamic conditions governing the optical temperature and chemical potential in nonlinear highly multimoded photonic systems, *Optics letters* **44**, 3936 (2019).
- [38] K. G. Makris, F. O. Wu, P. S. Jung, and D. N. Christodoulides, Statistical mechanics of weakly nonlinear optical multimode gases, *Optics Letters* **45**, 1651 (2020).
- [39] F. O. Wu, A. U. Hassan, and D. N. Christodoulides, Thermodynamic theory of highly multimoded nonlinear optical systems, *Nature Photonics* **13**, 776 (2019).
- [40] F. O. Wu, P. S. Jung, M. Parto, M. Khajavikhan, and D. N. Christodoulides, Entropic thermodynamics of nonlinear photonic chain networks, *Communications Physics* **3**, 1 (2020).
- [41] S. Chibbaro, G. Dematteis, and L. Rondoni, 4-wave dynamics in kinetic wave turbulence, *Physica D: Nonlinear Phenomena* **362**, 24 (2018).
- [42] M. Tanaka and N. Yokoyama, Numerical verification of the random-phase-and-amplitude formalism of weak turbulence, *Physical Review E* **87**, 062922 (2013).
- [43] H. Spohn, The phonon boltzmann equation, properties and link to weakly anharmonic lattice dynamics, *Journal of statistical physics* **124**, 1041 (2006).
- [44] R. Franzosi, Microcanonical entropy and dynamical measure of temperature for systems with two first integrals, *Journal of Statistical Physics* **143**, 824 (2011).
- [45] U. Levy and Y. Silberberg, Equilibrium temperatures of discrete nonlinear systems, *Physical Review B* **98**, 060303 (2018).
- [46] S. Chibbaro, G. Dematteis, C. Josserand, and L. Rondoni, Wave-turbulence theory of four-wave nonlinear interactions, *Physical Review E* **96**, 021101 (2017).

- [47] R. H. Kraichnan and D. Montgomery, Two-dimensional turbulence, *Reports on Progress in Physics* **43**, 547 (1980).
- [48] K. Baudin, A. Fusaro, K. Krupa, J. Garnier, S. Rica, G. Millot, and A. Picozzi, Classical rayleigh-jeans condensation of light waves: Observation and thermodynamic characterization, *Physical Review Letters* **125**, 244101 (2020).