Chapter 20
Statistical Mechanics of DNLS

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20.1 Introduction

In this section, we focus our attention on the long-time asymptotics of the system, aiming to understand the dynamics from the viewpoint of statistical mechanics. The study of the thermalization of the lattice for $T \geq 0$ was performed analytically as well as numerically in [1]. In that work, a regime in phase space was identified wherein regular statistical mechanics considerations apply, and hence, thermalization was 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" in the sense of statistical mechanics. The novel feature of these states was found to be that the energy spontaneously localizes in certain lattice sites forming breather-like excitations. Returning to statistical mechanics, such realizations are not possible (since the Hamiltonian is unbounded, as is seen by a simple scaling argument similar to the continuum case studied in [2]) unless the grand-canonical Gibbsian measure is refined to correct for the unboundedness. This correction was argued in [1] to produce a discontinuity in the partition function signaling a phase transition which was identified numerically by the appearance of the intrinsic localized modes (ILMs).

In our presentation below, we first elaborate on the semianalytical calculations of [1]. We then present direct numerical simulation results, supporting the theoretically analyzed scenario. We conclude our discussion with a number of more recent results, including a generalization of the considerations to higher dimensions and/or nonlinearity exponents, as well as other classes of related nonlinear lattices.

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20.2 Theoretical Results

To present the analysis of [1], it is convenient to use a slightly modified (yet equivalent, up to rescaling and gauge transformations) form of the DNLS

$$i\dot{u}_n + (u_{n+1} + u_{n-1}) + \nu|u_n|^2 u_n = 0. \tag{20.1}$$

In order to study the statistical mechanics of the system, we calculate the classical grand-canonical partition function $\mathcal{Z}$. Using the canonical transformation $u_n = \sqrt{A_n}\exp(i\phi_n)$, the Hamiltonian expressed as

$$H = \sum_n \left[\left(u_n^* u_{n+1} + u_n u_{n+1}^*\right) + \frac{\nu}{2}|u_n|^4 \right] \tag{20.2}$$

becomes

$$H = \sum_n 2\sqrt{A_n A_{n+1}}\cos(\phi_n - \phi_{n+1}) + \frac{\nu}{2}\sum_n A_n^2. \tag{20.3}$$

The partition function in this setting can be expressed as

$$\mathcal{Z} = \int_0^\infty \int_0^{2\pi} \prod_n d\phi_n dA_n \exp[-\beta(H + \mu P)] \,, \tag{20.4}$$

where the multiplier μ is analogous to the chemical potential introduced to ensure conservation of the squared l^2 norm $P = \sum_n |u_n|^2$. Straightforward integration over the phase variable ϕ_n yields

$$\mathcal{Z} = (2\pi)^N \int_0^\infty \prod_n dA_n I_0(2\beta\sqrt{A_n A_{n+1}}) \times \exp\left[-\beta \sum_n \left(\frac{\nu}{4}(A_n^2 + A_{n+1}^2) + \frac{\mu}{2}(A_n + A_{n+1}) \right) \right]. \tag{20.5}$$

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 [3, 4],

$$\int_0^\infty dA_n \, \kappa(A_n, A_{n+1}) \, y(A_n) = \lambda \, y(A_{n+1}), \tag{20.6}$$

where the kernel κ is

$$\kappa(x, z) = I_0\left(2\beta\sqrt{xz}\right) \exp\left[-\beta \left(\frac{\nu}{4}\left(x^2 + z^2\right) + \frac{\mu}{2}(x + z) \right) \right]. \tag{20.7}$$

Similar calculations were performed for the statistical mechanics of the ϕ^4 field [3, 4], and for models of DNA denaturation [5]. The partition function can, thus, be obtained as $\mathcal{Z} \simeq (2\pi\lambda_0)^N$, 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 purposes, the averaged energy density, $h = \langle H \rangle / N$, and the average excitation norm, $a = \langle P \rangle / N$, can be found as

$$a = -\frac{1}{\beta\lambda_0}\frac{\partial\lambda_0}{\partial\mu}, \quad h = -\frac{1}{\lambda_0}\frac{\partial\lambda_0}{\partial\beta} - \mu a. \tag{20.8}$$

The average excitation norm a can also be calculated as

$$a = (1/\mathcal{Z}) \int_0^\infty \prod_n dA_n \, A_n \exp\left[-\beta\,(H + \mu P)\right], \tag{20.9}$$

where the integral again can be calculated using the transfer integral technique [3, 4] 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. (20.5)). This shows that $p(A) = y_0^2(A)$ is the probability distribution function (PDF) for the amplitudes A. Subsequently, λ_0, y_0 were obtained numerically in [1]. However, two limits ($\beta \to \infty$ and $\beta \to 0$) can also be explored analytically. In particular, the minimum of the Hamiltonian is realized by a plane wave, $u_n = \sqrt{a}\exp i m\pi$, whose energy density is $h = -2a + \nu a^2/2$. This relation defines the zero temperature (or the $\beta = \infty$) line. For the high temperature limit, $\beta \ll 1$, the modified Bessel function in the transfer operator can be approximated to leading order, by unity which, in turn, reduces the remaining eigenvalue problem to the approximate solution,

$$y_0(A) = \frac{1}{\sqrt{\lambda_0}} \exp\left[-\frac{\beta}{4}\left(\nu A^2 + 2\mu A\right)\right]. \tag{20.10}$$

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

Figure 20.1 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 applicable and there is a one-to-one correspondence between (a, h) and (β, μ). Thus, within this range of parameter space the system thermalizes 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 was accomplished in [1] by introducing formally negative temperatures. However, the

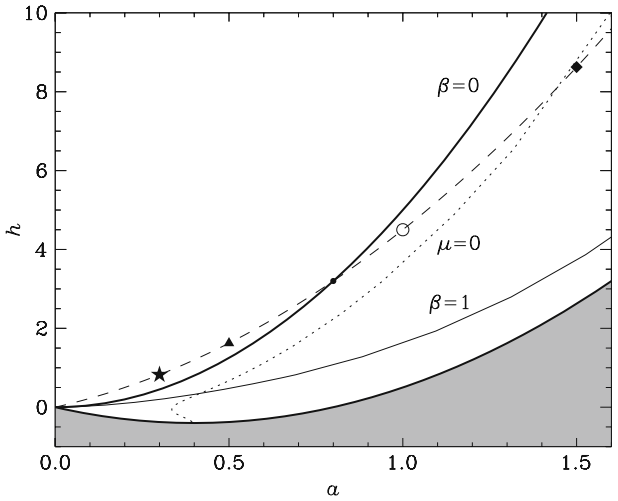

Fig. 20.1 From [1]: parameter space (a, h), where the *shaded area* is inaccessible. The *thick lines* represent, respectively, the $\beta = \infty$ and $\beta = 0$ cases and thus bound the Gibbsian regime. The *dashed line* represents the $h = 2a + \frac{\nu}{2}a^2$ curve along which the reported numerical simulations are performed (pointed by the symbols). The *dotted line* shows the locus of points where the chemical potential vanishes

partition function (20.4) is clearly not suited for that purpose since the constraint expressed in the grand-canonical form fails to bound the Hamiltonian of Eq. (20.2) from above. In all the alternative approaches of the study of negative temperatures a finite system of size N was thus considered. As suggested in [2] the grand-canonical ensemble can be realized using the modified partition function $\mathcal{Z}'(\beta, \mu') = \int \exp(-\beta(H + \mu' P^2)) \prod_n du_n du_n^*$, but this introduces long-range coupling and μ' will have to be of order $1/N$. Now β can be negative since $H + \mu' P^2$ 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, associated with 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.

In order to characterize the dynamics of both phases (above and below the $\beta = 0$ line) and to verify that the system relaxes to a thermalized state, numerical experiments were performed in [1]. The parameters (a, h) were restricted to the dashed line of Fig. 20.1, choosing an appropriate perturbed phonon as initial condition. The modulational instability of the latter [6] naturally gives rise to localized states. For these initial conditions, the important question is whether relaxation to equilibrium

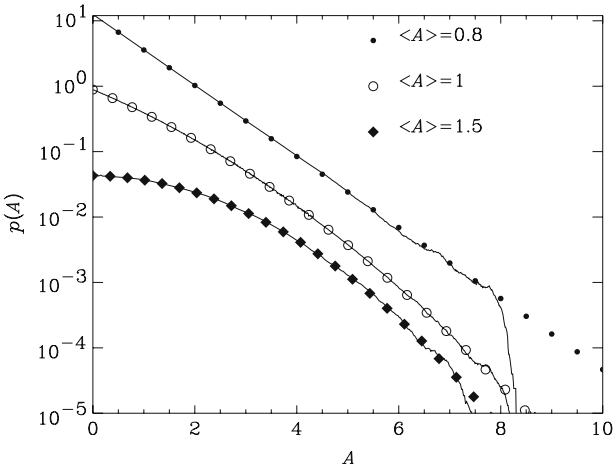

Fig. 20.2 From [1]: probability distribution of $A = |\psi|^2$ for three cases under (and on) the transition line. *The solid lines* show the results of simulations and the symbols are given by the transfer operator. Curves are vertically shifted to facilitate visualization

is really achieved and whether different qualitative behavior is indeed observed on the two sides of the $\beta = 0$ line.

Figure 20.2 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. 20.1). Since the initial condition is modulationally unstable, the energy density forms small localized excitations but their lifetime is not very long and, rapidly, a stationary distribution of the amplitudes A_n is reached (Fig. 20.2). Hence an equilibrium state is reached as predicted by means of the transfer-operator method.

The scenario is found to be very different when the energy and norm densities are above the $\beta = 0$ line. A rapid creation of ILMs due to the modulational instability is again observed and is accompanied by thermalization of the rest of the lattice. Once created however, these localized excitations remained mostly pinned and because the internal frequency increased with amplitude their coupling with the small-amplitude radiation was very small. This introduces a new time scale in the thermalization process necessitating symplectic integration for as long as $10^6 - 10^7$ time units in order to reach a stationary PDF. This was also qualitatively justified by the effective long-range interactions, introduced in the modified partition function, which produce stronger memory effects as one observes regimes in phase space which are further away from the transition line.

Typical distribution functions of the amplitudes are shown in Fig. 20.3. The presence of high-amplitude excitations is directly seen here. 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 signaled in the dynamics by the appearance of the strongly localized, persistent in the long-time asymptotics, ILMs.

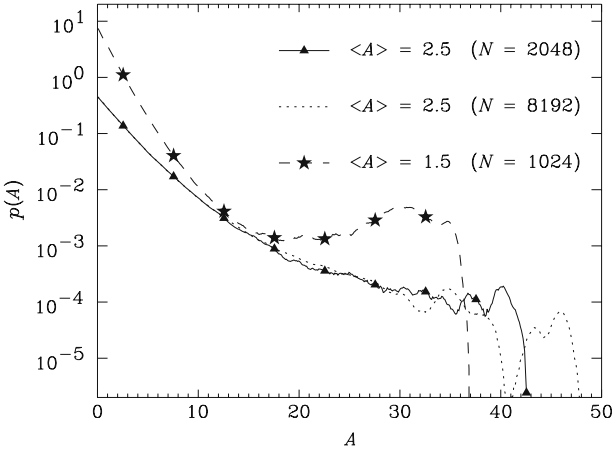

Fig. 20.3 From [1]: distribution of $A = |\psi|^2$ for parameters (h, a) above the transition line (*triangles* and *stars* as in Fig. 20.1.)

20.3 Recent Results

More recently, the statistical understanding of the formation of localized states and of the asymptotic dynamics of the DNLS equation has been addressed in the works of [7, 8].

The analysis of the former paper presented a complementary viewpoint to that of [1] which attempted for the first time to address the thermodynamics of the states within the localization regime. Assuming small-amplitude initial conditions, [7] argued that the phase space of the system can be divided roughly into two weakly interacting domains, one of which corresponds to the low-amplitude fluctuations (linear or phonon modes), while the other consists of the large-amplitude, localized mode nonlinear excitations. A remarkable feature of that work is that based on a simple partition of the energy $H = H_< + H_>$ and of the norm $P = P_< + P_>$, into these two broadly (and also somewhat loosely) defined fractions, one smaller than a critical threshold (denoted by $<$) and one larger than a critical threshold (denoted by $>$); it allows to compute thermodynamic quantities such as the entropy in this localization regime. In particular, one of the key results of [7] is that for a partition of K sites with large-amplitude excitations and $N - K$ sites with small-amplitude ones, it derives an expression for the total entropy (upon computing $S_<$, $S_>$, and a permutation entropy due to the different potential location of the K and $N - K$ sites). This expression reads

$$S = N\ln\Omega + \frac{P_>^2}{2E_>}\ln\Gamma, \tag{20.11}$$

where $\Omega = (4P_<^2 - E_<^2)/(4A_<(N - K))$ and $\Gamma = 2P_<N/P_>E_<$, while $K = P_>^2/(2E_>)$. While some somewhat artificial assumptions are needed to arrive at

the result of Eq. (20.11) [such as the existence of a cutoff amplitude radius R in phase space], nevertheless, the result provides a transparent physical understanding of the localization process. The contributions to the entropy stem from the fluctuations [first term in Eq. (20.11)] and from the high-amplitude peaks (second term in the equation). However, typically the contribution of the latter in the entropy is negligible, while they can absorb high amounts of energy. The underlying premise is that the system seeks to maximize its entropy by allocating the ideal amount of energy $H_<$ to the fluctuations. Starting from an initial energy $H_<$, this energy is decreased in favor of localized peaks (which contribute very little to the entropy). The entropy would then be maximized if eventually a single peak was formed, absorbing a very large fraction of the energy while consuming very few particles. Nevertheless, practically, this regime is not reached "experimentally" (i.e., in the simulations). This is because of the inherent discreteness of the system which leads to a pinning effect of large-amplitude excitations which cannot move (and, hence, cannot eventually merge into a single one) within the lattice. Secondly, the growth of the individual peaks, as argued in [7], stops when the entropy gain due to energy transfer to the peaks is balanced by the entropy loss due to transfer of power. While placing the considerations of [7] in a more rigorous setting is a task that remains open for future considerations, this conceptual framework offers considerable potential for understanding the (in this case argued to be infinite, rather than negative, temperature) thermal equilibrium state of coexisting large-amplitude localized excitations and small-amplitude background fluctuations.

On the other hand, the work of [8] extended the considerations of the earlier work of [1] to the generalized DNLS model of the form

$$i\dot{u}_n + (u_{n+1} + u_{n-1}) + |u_n|^{2\sigma} u_n = 0. \tag{20.12}$$

Our analytical considerations presented above are directly applicable in this case as well, yielding a partition function

$$\mathcal{Z} = (2\pi)^N \int_0^\infty \prod_n dA_n I_0(2\beta\sqrt{A_n A_{n+1}}) \times \tag{20.13}$$

$$\exp\left[-\beta \sum_n A_n \left(\mu + A_n^\sigma/(\sigma+1)\right)\right]. \tag{20.14}$$

This can be again directly evaluated in the high-temperature limit, where the modified Bessel function is approximated as $I_0 \approx 1$, as

$$\mathcal{Z} = (2\pi)^N \frac{1}{(\beta\mu)^N}\left(1 - \frac{\beta\Gamma(\sigma+1)}{(\beta\mu)^{\sigma+1}}\right), \tag{20.15}$$

with Γ denoting the Γ function. As a result, in this case,

$$a = \frac{1}{\beta\mu} - \frac{\Gamma(\sigma+1)}{\mu(\beta\mu)^{\sigma+1}} \tag{20.16}$$

$$h = \frac{\Gamma(\sigma+1)}{(\beta\mu)^{\sigma+1}} \tag{20.17}$$

and the relation between the energy density h and the norm density a is generalized from the $\sigma = 1$ limit as

$$h = \Gamma(\sigma+1)a^{\sigma+1}, \tag{20.18}$$

encompassing the parabolic dependence of that limit as a special case. It was once again confirmed in the setting of [8] that crossing this limit of $\beta = 0$ results in the formation of the large-amplitude, persistent few-site excitations. Another interesting observation made in [8] is that in this limit of $\beta = 0$, the coupling terms are inactive, hence, if additional dimension(s) are added to the problem, these do *not* affect the nature of the critical curve of Eq. (20.18). In that sense, the role of the dimensionality is different than the role of σ [with the latter being evident in Eq. (20.18]. This is to be contradistincted with the situation regarding the excitation thresholds or the thresholds for collapse, as discussed in Sect. III.2, whereby the dimensionality d and the exponent σ play an equivalent role, since it is when their product exceeds a critical value (in particular for $d\sigma \geq 2$) that such phenomena arise.

Finally, in the work of [8], the connection of these DNLS considerations with the generally more complicated Klein–Gordon (KG) models was discussed. Much of the above-mentioned phenomenology, as argued in [7], is critically particular to NLS-type models, due to the presence of the second conserved quantity, namely of the l^2 norm; this feature is absent in the KG lattices, where typically only the Hamiltonian is conserved. [8] formalizes the connection of DNLS with the KG lattices, by using the approximation of the latter via the former through a Fourier expansion whose coefficients satisfy the DNLS up to controllable corrections. Within this approximation, they connect the conserved quantity of the KG model to the ones of the DNLS model approximately reconstructing the relevant transition (to formation of localized states) criterion discussed above. However, in the KG setting this only provides a guideline for the breather formation process, as the conservation of the norm is no longer a true but merely an approximate conservation law. This is observed in the dynamical simulations of [8], where although as the amplitude remains small throughout the lattice the process is well described by the DNLS formulation, when the breathers of the KG problem grow, they violate the validity of the DNLS approximation and of the norm conservation; thus, a description of the asymptotic state and of the thermodynamics of such lattices requires further elucidation that necessitates a different approach. This is another interesting and important problem for future studies.

References

1. Rasmussen, K.Ø., Cretegny, T., Kevrekidis, P.G., Grønbech-Jensen, N.: Phys. Rev. Lett., **84**, 3740 (2000) 369, 370, 371, 372, 373, 374, 375
2. Lebowitz, J.L., Rose, H.A., Speer, E.R., J. Stat. Phys., **50**, 657 (1988). 369, 372
3. Krumhansl, J.A., Schrieffer, J.R.: Phys. Rev. B, **11**, 3535 (1975) 370, 371
4. Scalapino, D.J., Sears, M., Ferrell, R.A.: Phys. Rev. B, **6**, 3409 (1972) 370, 371
5. Dauxois, T., Peyrard, M., Bishop, A.R.: Physica, **66D**, 35 (1993) 371
6. Kivshar, Yu.S., Peyrard, M.: Phys. Rev. A, **46**, 3198 (1992) 372
7. Rumpf, B.: Phys. Rev E **69**, 016618 (2004) 374, 375, 376
8. Johansson, M., Rasmussen, K.Ø.: Phys. Rev. E **70**, 066610 (2004) 374, 375, 376