Coherent structures and statistical equilibrium states in a model of dispersive wave turbulence

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Abstract

We review a recent statistical equilibrium model of self-organization in a generic class of focusing, nonintegrable nonlinear Schrödinger (NLS) equations. Such equations provide natural prototypes for nonlinear dispersive wave turbulence. The primary result is that the statistically preferred state for such a system is a macroscopic solitary wave coupled with fine-scale turbulent fluctuations. The coherent solitary wave is a minimizer the Hamiltonian for a fixed particle number (or L^2 norm squared). The predictions of the statistical model are compared with direct numerical simulations of the NLS equation, and it is demonstrated that the model describes the long-time average behavior of solutions remarkably well. In particular, the statistical theory accurately captures both the coherent structure and the spectrum of the solution of the NLS system in the long-time state.

1 NLS and Soliton Turbulence

Turbulence in nonlinear media is often accompanied by the formation and persistence of lage-scale coherent structures. A well-known example is the formation of macroscopic quasi–steady vortices in a turbulent large Reynolds number two dimensional fluid[1, 2, 3, 5, 4]. Such phenomena also occur for many classical Hamiltonian systems, even though the dynamics of these systems is formally reversible [6]. In the present work, we shall focus our attention on a class of dispersive nonlinear wave equations whose solutions exhibit the tendency to form persistent coherent structures in the midst of small-scale turbulent fluctuations. This is the class of one-dimensional nonlinear Schrödinger (NLS) equations of the form

$$i\psi_t + \psi_{xx} + f(|\psi|^2)\psi \ = 0\,, \tag{1}$$

where $\psi(x,t)$ is a complex field. It is our primary purpose to develop a statistical model to characterize both the coherent structures and the turbulent fluctuations that emerge under the dynamics (1).

The NLS equation (1) describes the slowly-varying envelope of a wave train in a dispersive conservative system. Depending on the nonlinearity f, it models, among other things, gravity waves on deep water [7], Langmuir waves in plasmas [8], superfluid dynamics [10], and pulse propagation along optical fibers [9]. When $f(|\psi|^2) = \pm|\psi|^2$ and eqn. (1) is posed on the whole real line or on a bounded interval with periodic boundary conditions, the equation is completely integrable [11], but for other nonlinearities and/or boundary conditions, it is nonintegrable.

We shall assume throughout that eqn. (1) is posed in a bounded one dimensional interval with either periodic or homogeneous Dirichlet boundary conditions. We restrict our attention to attractive, or focusing, nonlinearities $f(f(a) \geq 0,\ f'(a) > 0)$ such that the dynamics described by (1) is nonintegrable, free of wave collapse, and admits stable solitary–wave solutions. The dynamics under these conditions has been referred to as *soliton turbulence* [12]. Such is the case for the important power law nonlinearities, $f(|\psi|^2) = |\psi|^s$, with $0 < s < 4$ (in the periodic case, $s \neq 2$ for nonintegrability) [13, 14], and also for the physically relevant saturated nonlinearities $f(|\psi|^2) = |\psi|^2/(1+|\psi|^2)$ and $f(|\psi|^2) = 1 - \exp(-|\psi|^2)$, which arise as corrections to the cubic nonlinearity for large wave amplitudes [15].

The NLS equation (1) may be cast in Hamiltonian form $i\psi_t = \delta H/\delta\psi^*$, where ψ^* is the complex conjugate of the field ψ, and H is the Hamiltonian:

$$H(\psi) = \int \left(|\psi_x|^2 - F(|\psi|^2)\right)\, dx\,. \tag{2}$$

The *potential* F is defined via the relation $F(a) = \int_0^a f(y)\,dy$. In additition to the Hamiltonian, the dynamics (1) conserves, the particle number integral

$$N(\psi) = \int |\psi|^2\, dx\,. \tag{3}$$

Equation (1) in one spatial dimension has solitary wave solutions of the form $\psi(x,t) = \phi(x)\exp(i\lambda^2 t)$, where ϕ satisfies the nonlinear eigenvalue equation:

$$\phi_{xx} + f(|\phi|^2)\phi - \lambda^2\phi = 0\,. \tag{4}$$

It has been argued [12, 16] that the solitary wave solutions play a prominent role in the long–time dynamics of (1), in that they act as *statistical attractors* to which the system relaxes. The numerical simulations in [12, 22, 17], as well as the simulations we shall present here, support this conclusion. Indeed, it is seen that for rather generic initial conditions the field ψ evolves, after a sufficiently long time, into a state consisting of a spatially localized coherent structure, which agrees quite closely with a solution of (4), coupled with small-scale turbulent fluctuations. At intermediate times the solution typically consists of a collection of these soliton-like structures, but as time evolves, the solitons undergo a succession of collisions in which the smaller soliton decreases in amplitude, while the larger one increases in amplitude. When solitons collide or interact, they shed radiation, or small–scale fluctuations. This process continues until eventually a single soliton of large amplitude survives amidst the turbulent background radiation. Figure 1 illustrates the evolution of the solution of (1) for the particular nonlinearity $f(|\psi|^2) = |\psi|$ and with periodic boundary conditions on the spatial interval $[0, 256]$.

2 A Statistical Mechanics Model

In modeling the long–time behavior of a nonintegrable Hamiltonian system such as NLS, it seems natural to appeal to the methods of equilibrium statistical mechanics. That such an approach may be relevant for understanding the asymptotic–time state for NLS has already been suggested in [12], although the thermodynamic arguments presented by these authors are formal and incomplete. Recently, Jordan *et al.* [17] have constructed a mean–field statistical theory to characterize the large–scale structure and the statistics of the small–scale fluctuations inherent in the asymptotic–time state of the NLS system

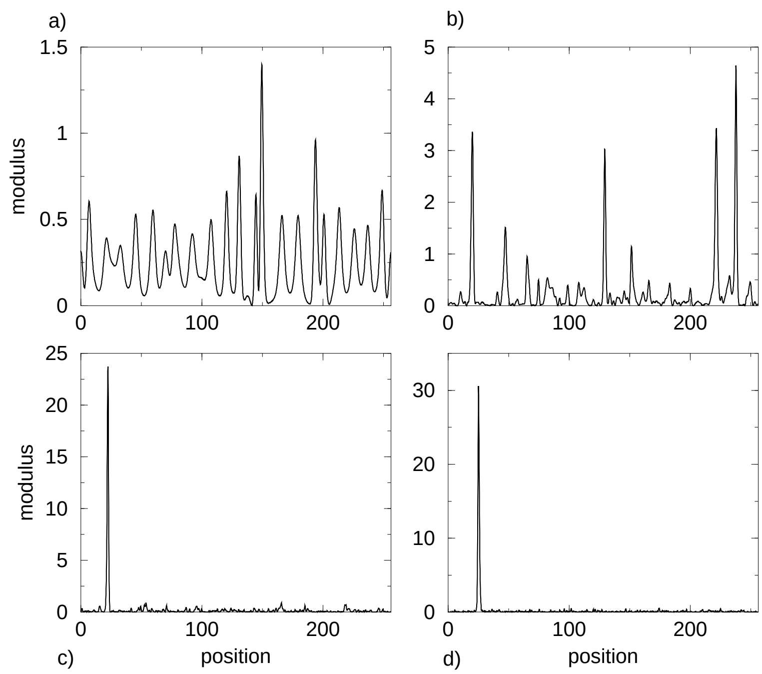

Figure 1: Profile of the squared modulus $|\psi|^2$ at four different times for the system (1) with nonlinearity $f(|\psi|^2) = |\psi|$ and periodic boundary conditions on the interval $[0, 256]$. The initial condition is $\psi(x, 0) = A$, with $A = 0.5$, plus a small random perturbation. The numerical scheme used to approximate the solution is the split-step Fourier method. The grid size is $dx = 0.125$, and the number of modes is $n = 2048$. a) $t = 50$ unit time: Due to the modulational instability, an array of soliton-like structures separated by the typical distance $l_i = 2\pi/\sqrt{A/2} = 4\pi$ is created; b) $t = 1050$ unit time: The solitons interact and coalesce, giving rise to a smaller number of solitons of larger amplitude; c) $t = 15050$: The coalescense process has ended. A single large soliton remains in a background of small–amplitude radiation. Notice that at $t = 55050$ unit time (d)), the amplitude of the fluctuations has diminished while the amplitude of the soliton has increased.

(1), and we shall review this theory and its predictions in the present article. The main conclusion of the theory is that the coherent state that emerges in the long–time limit is the ground state solution of equation (4). In other words, it is the solitary wave that minimizes the Hamiltonian H given the constraint $N = N^0$, where N^0 is the initial and conserved value of the particle number integral. This prediction is in accord with previous theories[12, 16], but the approach taken in [17] is different. Furthermore, as we shall see, the theory of [17] provides a definite interpretation to the notion set forth in the earlier works that it is "thermodynamically advantageous" for the NLS system to approach a coherent solitary wave structure that minimizes the Hamiltonian subject to fixed particle number. We now proceed to outline the statistical model developed in [17].

In order to develop a meaningful statistical theory, we begin by introducing a finite–dimensional approximation of the NLS equation (1). For ease of presentation, we will consider the NLS system with homogeneous Dirichlet boundary conditions on an interval Ω of length L. Our methods are readily modified to accommodate other boundary conditions, and we will consider below the predictions of the theory for periodic boundary conditions, as well. We remark that the techniques can easily be extended to higher dimensional NLS systems. Also, while we shall use a spectral truncation here, other discretization schemes would suit our purposes just as well.

Let $e_j(x) = \sqrt{2/L}\sin(k_j x)$ with $k_j = \pi j/L$, and for any function $g(x)$ on Ω denote by $g_j = \int_\Omega g(x)e_j(x)\,dx$ its jth Fourier coefficient with respect to the orthonormal basis $e_j, j = 1, 2, \cdots$. Define the functions $u^{(n)}(x,t) = \sum_{j=1}^n u_j(t)e_j(x)$ and $v^{(n)}(x,t) = \sum_{j=1}^n v_j(t)e_j(x)$, where the real coefficients $u_j, v_j, j = 1, \cdots, n$, satisfy the coupled system of ordinary differential equations

$$\begin{aligned} \dot{u}_j - k_j^2 v_j + \left(f((u^{(n)})^2 + (v^{(n)})^2)v^{(n)}\right)_j &= 0 \\ \dot{v}_j + k_j^2 u_j - \left(f((u^{(n)})^2 + (v^{(n)})^2)u^{(n)}\right)_j &= 0\,. \end{aligned} \tag{5}$$

Then the complex function $\psi^{(n)} = u^{(n)} + iv^{(n)}$ satisfies the equation

$$i\psi_t^{(n)} + \psi_{xx}^{(n)} + P^n(f(|\psi^{(n)}|^2)\psi^{(n)}) = 0\,,$$

where P^n is the projection onto the span of the eigenfunctions $e_1, \cdots, e_n$. This equation is a natural spectral approximation of the NLS equation (1), and it may be shown that its solutions converge as $n \to \infty$ to solutions of (1) [13, 18].

For given n, the system of equations (5) defines a dynamics on the $2n$–dimensional phase space $\mathbf{R}^{2n}$. This finite-dimensional dynamical system is a Hamiltonian system, with conjugate variables u_j and v_j, and with Hamiltonian

$$H_n = K_n + \Theta_n\,, \tag{6}$$

where

$$K_n = \frac{1}{2}\int_\Omega ((u_x^{(n)})^2 + (v_x^{(n)})^2)\,dx = \frac{1}{2}\sum_{j=1}^n k_j^2(u_j^2 + v_j^2)\,, \tag{7}$$

is the kinetic energy, and

$$\Theta_n = -\frac{1}{2}\int_\Omega F((u^{(n)})^2 + (v^{(n)})^2)dx\,, \tag{8}$$

is the potential energy. The Hamiltonian H_n is, of course, an invariant of the dynamics. The truncated version of the particle number

$$N_n = \frac{1}{2}\int_\Omega ((u^{(n)})^2 + (v^{(n)})^2)\,dx = \frac{1}{2}\sum_{j=1}^n (u_j^2 + v_j^2)\,, \tag{9}$$

is also invariant under the dynamics (5). The factor 1/2 is included in the definition of the particle number for mathematical convenience later on.

The Hamiltonian system (5) satisfies the Liouville property, which is to say that the measure $\prod_{j=1}^{n} du_j dv_j$ is invariant under the dynamics [19]. This property, together with the assumption of ergodicity of the dynamics, provides the usual starting point for a the statistical mechanics of a Hamiltonian system [20].

We introduce now a macroscopic description of the system (5) in terms of a probability density $\rho^{(n)}(u_1, \cdots, u_n, v_1 \cdots, v_n)$ on the $2n$–dimensional phase–space $\mathbf{R}^{2n}$. Thus, we seek a probability density that describes the statistical equilibrium state for the truncated dynamics. Following standard statistical mechanics and information theoretic practices [20, 21], we require this state to be the density $\rho^{(n)}$ on $2n$–dimensional phase space which maximizes the Gibbs-Boltzmann entropy

$$S(\rho) = -\int_{\mathbf{R}^{2n}} \rho \log \rho \prod_{j=1}^{n} du_j dv_j \,, \tag{10}$$

subject to constraints on the density associated with the invariance of the Hamiltonian and the particle number under the dynamics (5). The key to constructing the statistical model lies in choosing the appropriate constraints. Our choice is motivated by the observation from numerical simulations that, for a large number of modes n, in the long–time limit, the field $(u^{(n)}, v^{(n)})$ decomposes into two essentially distinct components: a large–scale coherent structure, and small–scale radiation, or fluctuations. The simulations illustrate that, as time increases, the amplitude of the fluctuations decreases, until eventually the contribution of the fluctuations to the particle number and the potential energy component of the Hamiltonian becomes negligible compared to the contribution from the coherent state. In the long-time limit, therefore, N_n and Θ_n are determined almost entirely by the coherent structure. We have checked that this effect becomes even more pronounced when the spatial resolution of the numerical simulations is improved. On the other hand, as the fluctuations exhibit rapid spatial variations, the amplitude of their gradient does not in general become negligible in the asymptotic time limit. In fact, the fluctuations typically make a significant contribution to the kinetic energy component K_n of the Hamiltonian. Fig. 2 demonstrates this effect quite clearly.

We denote by $\langle u_j \rangle$ and $\langle v_j \rangle$ the means of the coefficients u_j and v_j with respect the admissible ensemble $\rho^{(n)}$. The coherent state is identified with the mean–field pair $(\langle u^{(n)}(x) \rangle, \langle v^{(n)}(x) \rangle) = (\sum_{j=1}^{n} \langle u_j \rangle e_j(x), \sum_{j=1}^{n} \langle v_j \rangle e_j(x))$, and the fluctuations, or small-scale radiation inherent in the long–time state then correspond to the difference $(\delta u^{(n)}, \delta v^{(n)}) \equiv (u^{(n)} - \langle u^{(n)} \rangle, v^{(n)} - \langle v^{(n)} \rangle)$ between the state vector $(u^{(n)}, v^{(n)})$ and the mean–field vector. From the considerations of the preceding paragraph, it seems reasonable to require that the amplitude of the fluctuations of the field $\psi^{(n)}$ in the long-time state of the NLS system (5) vanish entirely (in some appropriate sense) in the continuum limit $n \to \infty$. Specifically, we shall make the following *vanishing of fluctuations hypothesis*:

$$\int_{\Omega} \left[\langle (\delta u^{(n)})^2 \rangle + \langle (\delta v^{(n)})^2 \rangle \right] dx \equiv \sum_{j=1}^{n} \left[\langle (\delta u_j)^2 \rangle + \langle (\delta v_j)^2 \rangle \right] \to 0 \,, \text{ as } n \to \infty \,. \tag{11}$$

Here, $\delta u_j = u_j - \langle u_j \rangle$ represents the fluctuations of the Fourier coefficient u_j about its mean value $\langle u_j \rangle$, and similarly for δv_j. It is important to emphasize that (11) is a hypothesis used to construct our statistical theory, and not a conclusion drawn from the theory itself.

The vanishing of fluctuations hypothesis immediately implies that, for n sufficiently large, the expectation $\langle N_n \rangle$ of the particle number is determined almost entirely by the mean $(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$. Furthermore, the hypothesis (11) implies that for n large, the expectation $\langle \Theta_n(u^{(n)}, v^{(n)}) \rangle$ of the potential energy is well approximated by $\Theta_n(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$, the potential energy contained in the mean. This may be verified by expanding the potential F about the mean $(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$ in equation (8), taking expectations, and noting that the vanishing of fluctuations hypothesis implies that

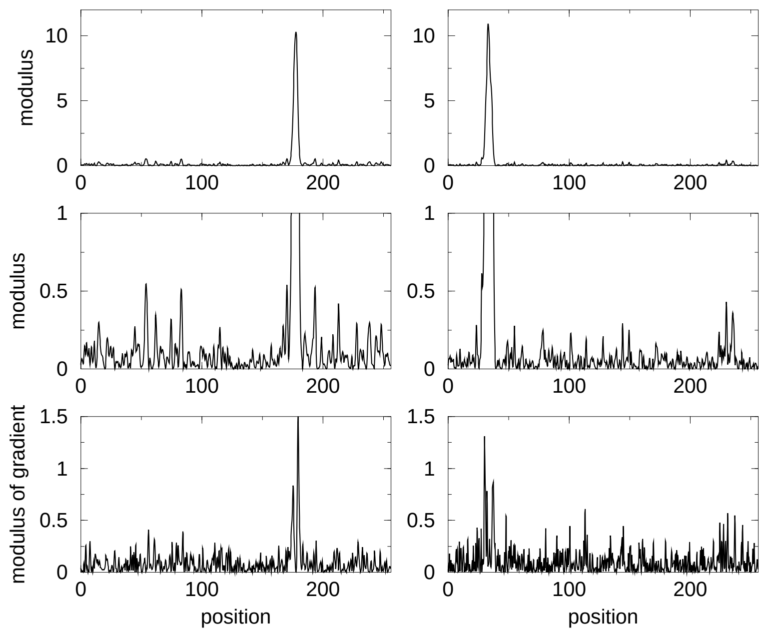

Figure 2: Numerical simulation for the saturated non-linearity $f(|\psi|^2) = |\psi|^2/(1 + |\psi|^2)$ and for periodic boundary conditions. The total number of modes is $n = 1024$ and the spatial grid size is $dx = 0.25$, so that the length of periodic interval is $L = 256$. Displayed are the squared modulus $|\psi|^2$ (first and second rows), and the squared modulus of the gradient of the field $|\psi_x|^2$ (third row) at unit times $t = 30,000$ (left) and $t = 220,000$ (right). The second row shows the same results as the first row, except that the we have restricted the range on the vertical axis in order to focus in on the the fluctuations of the field. The typical amplitude of the fluctuations of the field has decreased from $t = 30,000$ to $t = 220,000$ (second row), while the amplitude of the coherent structure has increased. On the other hand, the typical amplitude of the fluctuations of the gradient of the field has actually increased somewhat from $t = 30,000$ to $t = 220,000$.

$|\langle\Theta_n(u^{(n)}, v^{(n)})\rangle - \Theta_n(\langle u^{(n)}\rangle, \langle v^{(n)}\rangle)| = o(1)$ as $n \to \infty$ (see [17] for detailed calculations). It is important to recognize that the vanishing of fluctuations hypothesis does not imply that the contribution of the fluctuations to the expectation of the kinetic energy becomes negligible in the limit $n \to \infty$. This contribution is $(1/2)\sum_{j=1}^n k_j^2[\langle(\delta u_j)^2\rangle + \langle(\delta v_j)^2\rangle]$, which need not tend to 0 as $n \to \infty$, even if (11) holds. Thus, from these arguments, we conclude that for n sufficiently large, $\langle H_n\rangle \approx \frac{1}{2}\sum_{j=1}^n k_j^2(\langle u_j^2\rangle + \langle v_j^2\rangle) - \frac{1}{2}\int_\Omega F(\langle u^{(n)}\rangle^2 + \langle v^{(n)}\rangle^2)\,dx$. Based on these considerations, we impose the following *mean–field constraints* on the admissible probability densities $\rho^{(n)}$:

$$\begin{aligned} \tilde{N}_n(\rho^{(n)}) &\equiv \tfrac{1}{2}\textstyle\sum_{j=1}^n (\langle u_j\rangle^2 + \langle v_j\rangle^2) = N^0 \\ \tilde{H}_n(\rho^{(n)}) &\equiv \tfrac{1}{2}\textstyle\sum_{j=1}^n k_j^2(\langle u_j^2\rangle + \langle v_j^2\rangle) - \tfrac{1}{2}\int_\Omega F(\langle u^{(n)}\rangle^2 + \langle v^{(n)}\rangle^2)\,dx = H^0\,. \end{aligned} \tag{12}$$

Here, N^0 and H^0 are the conserved values of the particle number and the Hamiltonian, as determined from initial conditions. The statistical equilibrium states are then taken to be the probability densities $\rho^{(n)}$ on the phase–space $\mathbf{R}^{2n}$ that maximize the entropy (10) subject to the constraints (12). We shall refer to the constrained maximum entropy principle that determines the statistical equilibria as (MEP).

It has been proved in [17] that the solutions $\rho^{(n)}$ of (MEP) concentrate on the phase–space manifold on which $H_n = H^0$ and $N_n = N^0$ in the continuum limit $n \to \infty$, in the sense that $\langle N_n\rangle \to N^0$, $\langle H_n\rangle \to H^0$, and $\operatorname{var} N_n \to 0, \operatorname{var} H_n \to 0$ in this limit. Here, $\operatorname{var} W$ denotes the variance of the random variable W. This concentration property establishes a form of asymptotic equivalence between the mean–field ensembles $\rho^{(n)}$ and the microcanonical ensemble, which is the invariant measure concentrated on the phase–space manifold on which $H_n = H^0$ and $N_n = N^0$. This is a crucial result, because it is an accepted axiom of statistical mechanics that the microcanonical ensemble is the appropriate equilibrium ensemble for an isolated ergodic system [20]. Thus, this equivalence of ensembles property provides a strong theoretical justification for the mean–field statistical model, and it substantiates *a poseriori* the use of the vanishing of fluctuations hypothesis in constructing our statistical model. A detailed discussion of these issues can be found in [23].

3 Calculation and Analysis of Equilibrium States

The solutions $\rho^{(n)}$ of (MEP) are calculated by an application of the Lagrange multiplier rule

$$S'(\rho^{(n)}) = \mu\tilde{N}_n'(\rho^{(n)}) + \beta\tilde{H}_n'(\rho^{(n)})\,,$$

where β and μ are the Lagrange multipliers to enforce that the probability density $\rho^{(n)}$ satisfy the constraints (12). Fairly straightforward, but somewhat tedious, calculations calculation lead to the following expression for the maximum entropy distribution $\rho^{(n)}$[17]:

$$\rho^{(n)}(u_1,\ldots,u_n,v_1,\ldots,v_n) = \prod_{j=1}^n \rho_j(u_j,v_j)\,, \tag{13}$$

where, for $j = 1,\ldots,n$,

$$\rho_j(u_j,v_j) = \frac{\beta k_j^2}{2\pi}\exp\left\{-\frac{\beta k_j^2}{2}\left((u_j - \langle u_j\rangle)^2 + (v_j - \langle v_j\rangle)^2\right)\right\}\,, \tag{14}$$

with

$$\begin{aligned} \langle u_j\rangle &= \tfrac{1}{k_j^2}\left(f(\langle u^{(n)}\rangle^2 + \langle v^{(n)}\rangle^2)\langle u^{(n)}\rangle\right)_j - \tfrac{\mu}{\beta k_j^2}\langle u_j\rangle \\ \langle v_j\rangle &= \tfrac{1}{k_j^2}\left(f(\langle u^{(n)}\rangle^2 + \langle v^{(n)}\rangle^2)\langle v^{(n)}\rangle\right)_j - \tfrac{\mu}{\beta k_j^2}\langle v_j\rangle\,. \end{aligned} \tag{15}$$

It follows that, for each j, u_j and v_j are independent Gaussian random variables with means given by the nonlinear equations (15) and with variances

$$\text{var } u_j = \text{var } v_j = \frac{1}{\beta k_j^2} \,. \tag{16}$$

Note that var $u_j = \langle (\delta u_j)^2 \rangle$ by definition, and similarly for v_j. Notice also that, since the probability density $\rho^{(n)}$ is Gaussian and factors according to (13), the Fourier modes $u_j, v_j, j = 1, \cdots, n$, are statistically independent . Setting $\lambda = \mu/\beta$, the equations (15) imply that the complex mean–field $\langle \psi^{(n)} \rangle = \langle u^{(n)} \rangle + i \langle v^{(n)} \rangle$ is solution of

$$\langle \psi^{(n)} \rangle_{xx} + P^n \left(f(|\langle \psi^{(n)} \rangle|^2) \langle \psi^{(n)} \rangle \right) - \lambda \langle \psi^{(n)} \rangle = 0 \,. \tag{17}$$

This is obviously the spectral truncation of the eigenvalue equation (4) for the continuous NLS system (1). The important conclusion to be drawn from this is that the mean–field corresponds to a solitary wave solution of the NLS equation.

Since the maximum entropy distribution $\rho^{(n)}$ is required to satisfy the mean–field Hamiltonian constraint (12), we have from (13)–(17) that

$$H^0 = \frac{n}{\beta} + H_n(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle) \,. \tag{18}$$

The term $H_n(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$ is the Hamiltonian of the mean, while the term n/β represents the contribution to the kinetic energy from the random fluctuations. We see that the contribution of the fluctuations to the kinetic energy is equipartitioned among the n Fourier modes. From (18), we obtain the following expression for β in terms of the number of modes n and the Hamiltonian of the mean:

$$\beta = \frac{n}{H^0 - H_n(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)} \,. \tag{19}$$

We are now ready to establish an essential result: *The mean field $(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$ corresponding to the maximum entropy density $\rho^{(n)}$ is an absolute minimizer of the Hamiltonian H_n suject to the particle number constraint $N_n = N^0$.*

Indeed, using equations (13)–(19), we find after some algebraic manipulations that the entropy of any solution $\rho^{(n)}$ of (MEP) is

$$S(\rho^{(n)}) = C(n) + n \log \left(\frac{L^2 [H^0 - H_n(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)]}{n} \right) \,,$$

where $C(n) = n - \sum_{j=1}^{n} \log(j^2 \pi/2)$ depends only on the number of Fourier modes n. Clearly then, the entropy $S(\rho^{(n)})$ will be maximum if and only if the mean field pair $(\langle u^{(n)} \rangle, \langle v^{(n)} \rangle)$ realizes the minimum possible value of H_n over all fields $(u^{(n)}, v^{(n)})$ that satisfy the constraint $N_n(u^{(n)}, v^{(n)}) = N^0$. This is the desired conclusion.

The preceding argument reveals that, in statistical equilibrium the entropy is, up to additive and multiplicative constants, the logarithm of the the kinetic energy contained in the turbulent fluctuations about the mean state. This result, therefore, provides a precise interpretation to the notions set forth by Zakharov *et al.* [12] and Pomeau [16] that the entropy of the NLS system is directly related to the amount of kinetic energy contained in the small-scale fluctuations, and that it is "thermodynamically advantageous" for the solution of NLS to approach a ground state which minimizes the Hamiltonian for the given number of particles.

We now know that $H_n(\langle u^{(n)}\rangle, \langle v^{(n)}\rangle) = H_n^*$, where H_n^* is the minimum vale of H_n allowed by the particle number constraint $N_n = N^0$. Consequently, the Lagrange multiplier β is uniquely determined by (19):

$$\beta = \frac{n}{H^0 - H_n^*} \,. \tag{20}$$

The Lagrange multiplier λ (which also depends on n) is determined by the requirement that the mean $(\langle u^{(n)}\rangle, \langle v^{(n)}\rangle)$ minimizes the Hamiltonian H_n given the particle number constraint $N_n = N^0$.

Using eqns. (16) and (20), we may derive an exact expression for the contribution of the fluctuations to the expectation of the particle number. This is

$$\frac{1}{2}\sum_{j=1}^{n} \left[\langle(\delta u_j)^2\rangle + \langle(\delta v_j)^2\rangle\right] = \frac{H^0 - H_n^*}{n}\sum_{j=1}^{n}\frac{1}{k_j^2} = O(n^{-1})\,, \quad \text{as } n \to \infty\,. \tag{21}$$

In the derivation of the mean–field constraints (12), we assumed the vanishing of fluctuations condition (11). The calculation (21) shows, therefore, that the maximum entropy distributions $\rho^{(n)}$ indeed satisfy the hypothesis (11), and hence, that the mean–field statistical theory is consistent with the assumption that was made to derive it.

The statistical theory also provides predictions for the particle number and kinetic energy spectral densities, at least for the $2n$-dimensional spectrally truncated NLS system (5) with n large. In fact, we have the following prediction for the particle number spectral density

$$\langle|\psi_j|^2\rangle = |\langle\psi_j\rangle|^2 + \frac{H^0 - H_n^*}{n k_j^2}\,, \tag{22}$$

where we have used the identity $\psi_j = u_j + i v_j$, and eqns. (16) and (20). The first term on the right hand side of (22) is the contribution to the particle number spectrum from the mean, and the second term is the contribution from the fluctuations. As the mean field is a smooth solution of the ground-state equation, its spectrum decays rapidly, so that for $j >> 1$, we have the approximation $\langle|\psi_j|^2\rangle \approx (H^0 - H_n^*)/(n k_j^2)$. The kinetic energy spectral density is obtained simply by multiplying eqn. (22) by k_j^2. In partcular, we have the prediction that the kinetic energy arising from the fluctuations is equipartitioned among the n spectral modes, with each mode contributing the amount $(H^0 - H_n^*)/n$.

While we have focused on homogeneous Dirichlet boundary conditions so far, it is straightforward to modify the statistical theory to accomodate periodic boundary conditions on an interval of length L, say. In this case, it is convenient to write the spectrally truncated complex field $\psi^{(n)}$ as

$$\psi^{(n)} = \sum_{j=-n/2}^{n/2} \psi_j \exp(i k_j x)\,,$$

for n an even positive integer, where $k_j = 2\pi j/L$. The predictions of the statistical theory remain the same as in the case of Dirichlet boundary conditions. Namely, the mean field $\langle\psi^{(n)}\rangle$ is a minimizer of the Hamiltonian H_n given the particle number constraint $N_n = N^0$, and the particle number spectrum satisfies (22) for $j \neq 0$. The Fourier coefficient ψ_0 may be consistently chosen to be deterministic (i.e., var $\psi_0 = 0$ and $\langle\psi_0\rangle \equiv \psi_0$), to eliminate the ambiguity arising from the 0 mode.

4 Comparisons with Numerical Simulations

Our primary purpose in this section is to compare the predictions of the mean-field statistical theory described above with the results of high resolution direct numerical simulations of NLS. In particular, we wish to examine how closely the coherent structure and the spectra predicted by the statistical theory agree with those observed in long-time numerical simulations. Here, we will present numerical results primarily for periodic boundary conditions and for the focusing power law nonlinearity $f(|\psi|^2) = |\psi|$. That is, we shall solve numerically the particular NLS equation

$$i\psi_t + \psi_{xx} + |\psi|\psi = 0\,, \tag{23}$$

on a periodic interval of length L. This nonlinearity offers a nice compromise between the focusing effect and nonlinear interactions. For weaker nonlinearities (such as the saturated ones), the interaction between modes is weak, and the time required to approach an asymptotic equilibrium state is quite long. For stronger nonlinearities, the solitary wave structures that emerge exhibit narrow peaks of large amplitude, and consequently, higher spatial resolution is required in the numerical simulations. We have performed elsewhere similar numerical experiments for different focusing nonlinearities and for Dirichlet boundary conditions, and we have observed that the general qualitative features of the long-time dynamics are unaltered by such changes (see, for example [17, 22]).

On the whole real line, the nonlinear Schrödinger equation (23) has solitary wave solutions of the form $\psi(x,t) = \phi(x)e^{i\lambda^2 t}$, with

$$\phi(x) = \frac{3\lambda^2}{2\cosh^2(\frac{\lambda(x-x_0)}{2})} \tag{24}$$

The particle number N and the Hamiltonian H of these solutions are determined by the parameter λ via the relationships $N = 6\lambda^3$ and $H = -\frac{18}{5}\lambda^5$. For a given value of the particle number N, the solitary wave (24) is the global minimizer of the Hamiltonian H. Of course, the solitary wave solutions for the equation (23) on a finite interval, as well as those for the spectrally-truncated version (5), differ from the solution (24) over the infinite interval. However, as the solitary waves (24) exhibit exponential decay, such differences can be neglected for all practical purposes if the spatial interval is large enough and if the number of modes is sufficiently large. We shall be comparing the coherent structures observed in the numerical simulations to the expression (24).

In our numerical simulations, the initial condition is taken to be the spatially homogeneous solution (condensate) $\psi(x) = A$ (A constant) coupled with a small spatially uncorrelated random perturbation. By choosing different realizations of the initial random perturbation, we may perform an ensemble average over different initial conditions for a given A (and therefore for fixed N^0 and H^0). The initial conditions we consider here may be thought of as being far away from the expected statistical attractor described by the maximum entropy probability density $\rho^{(n)}$, as the spectrum of the condensate differs considerably from the predicted statistical equilibrium spectrum (22). As we shall see, the numerical simulations provide convincing evidence that the solutions of the spectrally truncated NLS system converge in the long-time limit to a state that may be considered as statistically steady, and whose average fetures are very well described by the mean-field statistical ensemble.

The numerical scheme that we use for solving (23) is the well-known split-step Fourier method for a given number n of Fourier modes. Throughout the duration of the simulations, the relative error in the particle number is kept at less than 10^{-6} percent, and the relative error in the Hamiltonian is no greater than 10^{-2} percent. Note that these numerical simulations, which necessarily pertain to a finite number of Fourier modes, provide a perfect setting for comparisons with the statistical model discussed above.

Figure 1 demonstrates that the dynamics can be roughly decomposed into three stages: in the first stage, illustrated in Fig. 1a, the modulational instability creates an array of soliton-like structures separated by a typical distance $l_i = 2\pi/k_i$ associated with most unstable wave number k_i. The second stage is characterized by the interaction and coalescence of these solitons. In this stage, the number of solitons decreases, while the amplitudes of the surviving solitons increase. Eventually a single soliton of large amplitude persists amongst a sea of small-amplitude background radiation (Figs. 1b and c).

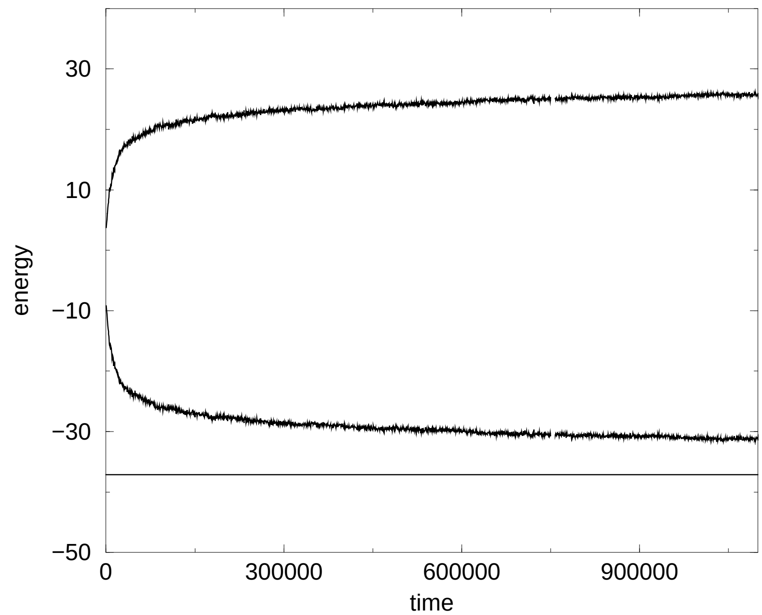

Figure 3: Time evolution of the kinetic (upper curve) and the potential (middle curve) energies. The kinetic energy is increasing and consequently the potential energy is decreasing, *in accord* with the statistical theory developed above. The lower line indicates the potential energy of the solitary wave that contains all the particles of the system. The curves are obtained from an ensemble average over 16 initial conditions for $n = 512$. The length of the system is $L = 128$, and the (conserved) values of the particle number and the Hamiltonian are, respectively, $N^0 = 20.48$ and $H^0 = -5.46$.

During the final stage of the dynamics, the surviving large-scale soliton interacts with the small-scale fluctuations. As time increases, the amplitude of the soliton increases, while the amplitude of the radiation decreases (note the changes from Fig. 1c to Fig. 1d). In this stage of the dynamics, the mass (or number of particles) is gradually transferred from the small-scale fluctuations to the large-scale coherent soliton. Eventually, the coherent structure attains a maximum amplitude, and subsequently, the coherent soliton and small-scale radiation appear to coexist in a statistically steady state.

Further evidence of the tendency of the solution of the NLS system (23) to approach a state of statistical equilibrium is furnished by the time evolution of the kinetic and potential energies (see Fig. 3). The sum of these two quantities is the Hamiltonian, and, therefore, remains constant in time. We observe, however, that the kinetic energy increases monotonically, and, consequently, the potential energy decreases monotonically as time goes on. The initial time period where these quantities evolve most rapidly (say $t < 20000$) corresponds to the first two stages of the dynamics described above, in which the modulational instability creates an array of soliton-like structures which then coalesce into a single coherent soliton. After the coalescence has ended, the kinetic (potential) energy increases (decreases) very slowly to its saturation value. In the process, fluctuations develop on increasingly finer spatial scales, which accounts for the gradual increase of kinetic energy. Simultaneously, the surviving soliton slowly absorbs mass from the background fluctuations, thereby increasing the magnitude of the contribution to the potential energy from the coherent structure. In the long-time limit, the soliton accounts for the vast majority of the potential energy, while the fluctuations make a nonnegligible contribution to the kinetic energy.

The statistical theory described above provides a prediction for the expected value of the kinetic energy K_n in statistical equilibrium for a given number of modes n. This is $\langle K_n \rangle = K_n(\langle \psi^{(n)} \rangle) + H^0 - H_n^*$, which follows directly upon multiplying eqn. (22) by k_j^2 and summing over j. The first term in this expression for $\langle K_n \rangle$ is the contribution to the mean kinetic energy from the coherent soliton structure which minimizes the Hamiltonian H_n subject to the particle number constraint $N_n = N^0$. The second term in $\langle K_n \rangle$ is the contribution to the expectation of the kinetic energy from the fluctuations. H_n^* is the minimum value of H_n given the particle number constraint. As $n \to \infty$, we see that $\langle K_n \rangle$ converges to $K(\psi^\infty) + H^0 - H^*$, where ψ^∞ is the minimizer of the Hamiltonian H given the particle number constraint $N = N^0$ for continuous NLS system on the interval $[0, L]$, and $H^* = H(\psi^\infty)$. Approximating $K(\psi^\infty)$ and $H(\psi^\infty)$ by $K(\phi)$ and $H(\phi)$, where ϕ is the solitary wave on the real line whose particle number is N^0, we obtain for the setting considered in Fig. 3 the large n estimates $K_n(\langle \psi^{(n)} \rangle) \approx 9.2, H^0 - H_n^* \approx 22.4$, and therefore, $\langle K_n \rangle \approx 31.6$. Also, according to the statistical theory, the expected value $\langle \Theta_n \rangle$ of the potential energy in statistical equilibrium should converge as $n \to \infty$ to $\Theta(\psi^\infty)$. Approximating this by $\Theta(\phi)$, with ϕ as above, we have the estimate $\langle \Theta_n \rangle \approx -37.1$, which we expect to be accurate for sufficiently large n. We see that the kinetic (potential) energy of the numerical solution is bounded above (below) by the estimate based on the statistical theory. As expected, the theoretically predicted value of the average kinetic energy for a finite number of modes is not attained. The reason for the difference is that a nonzero amount of the particle number and the potential energy are actually contained in the background radiation (according to the statistical theory, the expected contribution of the fluctuations to these quantities is $O(1/n)$, where n is the number of spectral modes –this follows from (22) [17]). It may be checked [22] that when the spatial resolution is improved, the contributions of the radiation to the particle number and the potential energy decrease, and the saturation values of the kinetic and potential energy attained in the numerical simulations approach more closely the predicted statistical equilibrium averages of these quantities.

Figures 1 and 3 offer evidence that, for a given (large) number of modes n, the dynamics converges in the long-time limit when to a state consisting of a large-scale coherent soliton, which accounts for all but a small fraction of the particle number and the potential energy integrals, coupled with small-scale radiation, or fluctuations, which account for the discrepency between the total kinetic energy and the kinetic energy contained in the coherent structure. In fact, eqn. (22) suggests that, in the long–time limit, the coherent structure and the background radiation exist in balance (or in statistical equilibrium) with each other through the equipartition of the kinetic energy of the fluctuations. In Fig. 4, we display the particle number spectral density $|\psi_k|^2$ as a function of the wave number k for a long time run, where ψ_k is the Fourier transform of the field ψ. This spectrum is obtained through an ensemble average over 16 initial conditions, and a time average over the final 1000 time units for each run. For comparison, we display in this figure the spectrum of the solitary wave (24) whose particle number is equal to conserved value of the particle number for the simulation. There is both a qualitative and quantitative agreement between the spectrum of this solitary wave solution and the small wavenumber portion of the spectrum arising from the numerical simulations. This is in agreement with the statistical theory, which predicts that the coherent structure should coincide with this solitary wave (in the limit $n \to \infty$). For larger wavenumbers, the spectrum of the numerical solution is dominated by the small scale fluctuations. We have indicated on the graph the large wavenumber spectrum predicted by the statistical theory. This prediction comes from the second expression on the right hand side of eqn. (22), except that we have approximated the minimum value H_n^* of the Hamiltonian for the spectrally truncated system by the Hamiltonian H^* of the above-mentioned solitary wave solution for the continuum system. We observe a good qualitative agreement with the predicted $\propto k^{-2}$ spectrum, corresponding to the equipartition of kinetic energy amongst the small-scale fluctuations. Furthermore, there is an excellent quantitative agreement between the numerical results and the formula (22) for large k.

As mentioned above, the numerical spectrum shown in Fig. 4 arises from an ensemble average over long time and over different initial conditions (with the same values of the particle number and the Hamiltonian). Under the assumption that the dynamics is ergodic, such an average should coincide

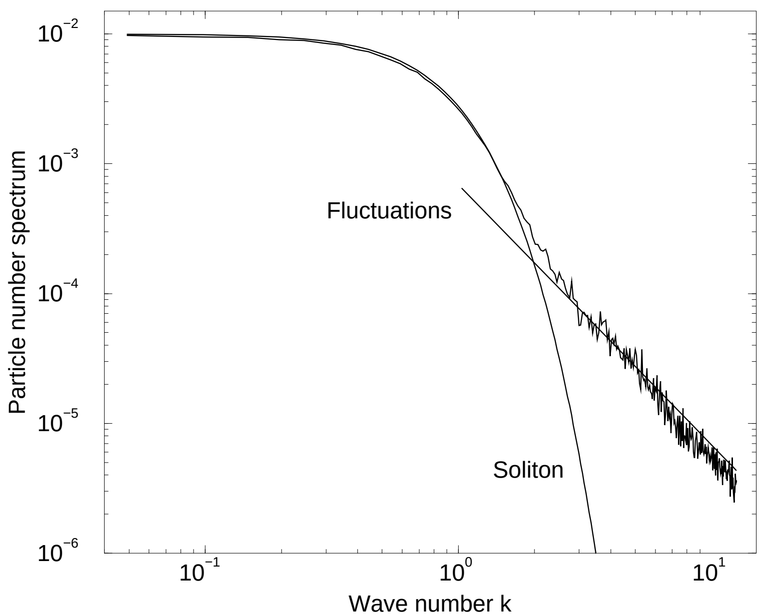

Figure 4: Particle number spectral density $|\psi_k|^2$ as a function of k for $t = 1.1 \times 10^6$ unit time (upper curve). The lower curve (smooth one) is the particle number spectral density for the solitary wave that contains all the particles of the system. The straight line drawn for large k corresponds to the statistical prediction (22) for the spectral density for large wavenumbers. The numerical simulation has been performed with $n = 512$, $dx = 0.25$, $N^0 = 20.48$ and $H^0 = -5.46$.

with an average with respect to the microcanonical ensemble for the spectrally truncated NLS system [20]. Since it has been shown that the the mean–field statistical ensembles $\rho^{(n)}$ constructed above concentrate on the microcanonical ensemble in the continuum limit $n \to \infty$ (see Theorem 3 of reference [17]), averages with respect to $\rho^{(n)}$ for large n should agree with the ensemble average of the numerical simulations over initial conditions and time, assuming ergodicity of the dynamics. While we have not shown that the dynamics is ergodic, we have, in fact, demonstrated a convincing agreement between the predictions of the mean–field ensembles $\rho^{(n)}$ and the results of direct numerical simulations. In [22], we have also compared the long-time saturation values of the quantities

$$S_m(\psi^{(n)}) = \sum k_j^{2m} |\psi_j|^2 ,$$

attained in numerical simulations with the predicted statistical equilibrium averages under the mean–field maximum entropy ensemble, where m is a positive integer. Once again, a close agreement between the numerical and theoretically predicted values is found.

5 Conclusions

The primary purpose of the present work has been to test the predictions of a mean–field statistical model of self-organization in a generic class of nonintegrable focusing NLS equations defined by eqn. (1). This statistical theory, which has been summarized above, was originally developed and analyzed in [17]. In fact, we have demonstrated a remarkable agreement between the predictions of the statistical theory and the results of direct numerical simulations of the NLS system. There is a strong qualitative and quantitative agreement between the mean field predicted by the statistical theory and the large-scale coherent structure observed in the long-time numerical simulations. In addition, the statistical model accurately predicts the the long-time spectrum of the numerical solution of the NLS system. The main conclusions we have reached are 1) The coherent structure that emerges in the asymptotic time limit is the solitary wave that minimizes the system Hamiltonian subject to the particle number constraint $N = N^0$, where N^0 is the given (conserved) value of N, and 2) The difference between the conserved Hamiltonian and the Hamiltonian of the coherent state resides in Gaussian fluctuations equipartitioned over wavenumbers. Further comparisons between the predictions of the statistical theory and the results of direct numerical simulations of NLS may be found in [22].

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