Condensation of Classical Nonlinear Waves

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We study the formation of a large-scale coherent structure (a condensate) in classical wave equations by considering the defocusing nonlinear Schrödinger equation as a representative model. We formulate a thermodynamic description of the classical condensation process by using a wave turbulence theory with ultraviolet cutoff. In three dimensions the equilibrium state undergoes a phase transition for sufficiently low energy density, while no transition occurs in two dimensions, in complete analogy with standard Bose-Einstein condensation in quantum systems. On the basis of a modified wave turbulence theory, we show that the nonlinear interaction makes the transition to condensation subcritical. The theory is in quantitative agreement with the numerical integration of the nonlinear Schrödinger equation.

The problem of self-organization in conservative systems has generated much interest in recent years. For infinite dimensional Hamiltonian systems like *classical* wave fields, the relationship between formal reversibility and actual dynamics can be rather complex. In integrable systems, such as the 1D nonlinear Schrödinger (NLS) equation, the dynamics is essentially periodic in time, reflecting the underlying regular phase-space structure of nested tori. This recurrent behavior is broken in nonintegrable systems, where the dynamics is in general governed by an irreversible process of diffusion in phase space [1]. In this respect, an important insight was obtained from numerical simulations of *solitons* in the focusing, nonintegrable NLS equation [2]. These studies revealed that the nonlinear wave would generally evolve to a state containing a large-scale coherent localized structure, i.e., solitary-wave, immersed in a sea of small-scale turbulent fluctuations. The solitary wave is a "statistical attractor" for the system, while the fluctuations contain, in principle, all information necessary for time reversal. Importantly, the solitary-wave solution minimizes the energy (Hamiltonian), so the system actually relaxes towards the state of lowest energy [2]. Only recently has a statistical description of this self-organization been developed [3,4]. Remarkably, when such systems are constrained by an additional invariant (e.g., the mass), the increase in entropy of small-scale turbulent fluctuations *requires* the formation of coherent structures to "store" this invariant [4], so that it is thermodynamically advantageous for the system to approach the ground state which minimizes the energy [2].

We consider here the *defocusing* regime of the NLS dynamics, which is also relevant to the description of thermal Bose gases [5–7]. This regime would be characterized by an irreversible evolution of the system to a homogenous plane-wave [8–11], which can be described by weak-turbulence theory [12]. This evolution is consistent with the scenario discussed above [2–4], because a plane wave minimizes the energy (Hamiltonian) in the defocusing case. Thus the NLS equation should exhibit a condensation process, a feature that has recently been confirmed in the context of thermal Bose fields using 3D numerical simulations of the NLS equation [6,7].

In this Letter we formulate a thermodynamic description of this condensation process. We show that the 3D NLS equation exhibits a *subcritical* condensation process. Its thermodynamic properties are analogous to those of Bose-Einstein condensation in quantum systems, despite the fact that this wave system is completely *classical.* We use a kinetic theory of the NLS equation in our analysis. We introduce a frequency cutoff to regularize the ultraviolet catastrophe inherent to ensembles of classical waves (Rayleigh-Jeans paradox). We find that in 2D the NLS equation does not undergo condensation in the thermodynamic limit, in complete analogy with a uniform, ideal Bose gas. The significance of this result is that the system irreversibly evolves to a state of equilibrium (maximum entropy) *without generating a coherent structure minimizing the Hamiltonian.* This contrasts with the general rule outlined in [2–4,11].

Given the universality of the NLS equation in nonlinear science, this condensation process could stimulate interesting new experiments in various branches of physics. Nonlinear optics is a natural context where classical wave condensation may be observed and studied experimentally. Moreover, the formal reversibility of the condensation process could be demonstrated by means of an optical phase-conjugation experiment. Additionally, wave condensation could be relevant to hydrodynamic surface waves [13], given recent progress on measurements of Zakharov's spectra.

We consider the normalized defocusing NLS equation in D spatial dimensions for the complex function ψ:

$$i\partial_t\psi = -\Delta\psi + |\psi|^2\psi, \tag{1}$$

where Δ is the D dimensional Laplacian. This equation describes the evolution of defocusing interacting waves through the cubic nonlinear term. The dynamics conserves the mass (particle number) $N = \int |\psi|^2 d^D x$, and the total energy $H = \int (|\nabla\psi|^2 + \frac{1}{2}|\psi|^4) d^D x$.

We address the dynamical formation of the condensate starting from a nonequilibrium stochastic initial condition for the wave ψ, which we take to be of zero mean and statistically homogeneous. In spite of the formal reversibility of the NLS equation, the nonlinear wave ψ is expected to exhibit an *irreversible* evolution towards thermal equilibrium, as a result of an effective diffusion process in phase space. The salient properties of this evolution may be described by weak-turbulence theory. For most purposes this is equivalent to the random phase approximation (assumption of quasi-Gaussian statistics) [12]. This approximation breaks the time reversal symmetry of the NLS equation, which allows one to derive an irreversible kinetic equation for the averaged wave spectrum [12] [here $\langle a_{\boldsymbol{k}_1} a^*_{\boldsymbol{k}_2}\rangle = n_{\boldsymbol{k}_1}\delta^{(D)}(\boldsymbol{k}_1 - \boldsymbol{k}_2)$, $a_{\boldsymbol{k}}$ being the Fourier transform of ψ defined by $a_{\boldsymbol{k}}(t) = \int \psi(\boldsymbol{x}, t) e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} d^D x$]:

$$\partial_t n_{\boldsymbol{k}_1}(t) = \int d^D k_2 d^D k_3 d^D k_4 W_{k_1,k_2;k_3,k_4}(n_{\boldsymbol{k}_3} n_{\boldsymbol{k}_4} n_{\boldsymbol{k}_1} + n_{\boldsymbol{k}_3} n_{\boldsymbol{k}_4} n_{\boldsymbol{k}_2} - n_{\boldsymbol{k}_1} n_{\boldsymbol{k}_2} n_{\boldsymbol{k}_3} - n_{\boldsymbol{k}_1} n_{\boldsymbol{k}_2} n_{\boldsymbol{k}_4}), \tag{2}$$

where the collision term $\mathrm{Coll}[n_{\boldsymbol{k}}]$ [right-hand side of Eq. (2)] provides a kinetic description of the four-wave interaction, with $W_{k_1,k_2;k_3,k_4} = \frac{4\pi}{(2\pi)^D}\delta^{(D)}(\boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}_3 - \boldsymbol{k}_4)\delta^{(1)}(k_1^2 + k_2^2 - k_3^2 - k_4^2)$ [12]. Like Boltzmann's equation, Eq. (2) conserves the mass, $N = V\int n_{\boldsymbol{k}}(t) d^D k$, and the kinetic energy, $E = V\int k^2 n_{\boldsymbol{k}}(t) d^D k$. V is the system volume in $D = 3$ and the area in $D = 2$. It has an H theorem for entropy growth $dS/dt \geq 0$, where $S(t) = \int \ln(n_{\boldsymbol{k}}) d^D k$ is the nonequilibrium entropy. The kinetic Eq. (2) then describes an irreversible evolution of the wave spectrum towards the Rayleigh-Jeans *equilibrium* distribution [12]:

$$n_k^{\mathrm{eq}} = \frac{T}{k^2 - \mu}, \tag{3}$$

where T and μ (≤ 0) are, by analogy with thermodynamics, the temperature and the chemical potential, respectively. The spectrum (3) is Lorentzian and the characteristic correlation length of the wave ψ is $\lambda_c \propto 1/\sqrt{-\mu}$.

The distribution (3) realizes the maximum of the entropy $S[n_{\boldsymbol{k}}]$ and vanishes exactly the collision term, $\mathrm{Coll}[n_k^{\mathrm{eq}}] = 0$. However, it is important to note that Eq. (3) is only a *formal* solution, because it does not lead to converging expressions for the energy E and the mass N in the short-wavelength limit $k \to \infty$. To regularize this unphysical divergence, we introduce an ultraviolet cutoff k_c; i.e., we assume $n_{\boldsymbol{k}}(t) = 0$ for $k > k_c$. Note that this cutoff arises naturally in numerical simulations through the spatial discretization of the NLS equation, and manifests itself in real physical systems through viscosity or diffusion effects at the microscopic scale [12].

To begin let us analyze the equilibrium distribution (3) in 3D. From energy and mass conservation one gets

$$\frac{N}{V} = 4\pi T k_c\left[1 - \frac{\sqrt{-\mu}}{k_c}\arctan\left(\frac{k_c}{\sqrt{-\mu}}\right)\right], \tag{4}$$

$$\frac{E}{V} = \frac{4\pi T k_c^3}{3}\left[1 + 3\frac{\mu}{k_c^2} + 3\left(\frac{-\mu}{k_c^2}\right)^{3/2}\arctan\left(\frac{k_c}{\sqrt{-\mu}}\right)\right]. \tag{5}$$

These equations are interpreted as follows. The initial nonequilibrium state of the field ψ has mass N and energy E. The wave spectrum then relaxes to the equilibrium distribution (3), whose temperature T and chemical potential μ are determined by Eqs. (4) and (5). A given pair (N, E) then determines a unique pair (T, μ). Equation (4) reveals that μ tends to zero, i.e., λ_c diverges to infinity, for a nonvanishing temperature T (keeping N/V constant), or a finite density N/V (keeping T constant). By analogy with the Bose-Einstein transition in quantum systems, this reveals the existence of a condensation process. The same conclusion follows from analyzing the energy per particle E/N. There exists a nonvanishing critical energy per particle $E_{\mathrm{tr}}/N = k_c^2/3$ such that $\mu = 0$. Dividing (5) by (4), one gets $(E - E_{\mathrm{tr}})/(Nk_c^2) = \pi\sqrt{-\mu}/(6k_c) + \mathcal{O}(-\mu/k_c^2)$. Decreasing the energy per particle effectively cools the system, and one reaches a finite threshold E_{tr}, below which condensation occurs.

A similar analysis in 2D readily gives $N/V = \pi T\ln(1 - k_c^2/\mu)$ and $E/N = \mu + k_c^2/\ln(1 - k_c^2/\mu)$. In this case μ reaches 0: (i) for a vanishing temperature T (N/V constant), (ii) for a diverging density N/V (T constant), (iii) for a vanishing energy per particle E/N. It follows that condensation no longer takes place in 2D, a feature that has been confirmed by numerical simulations of the NLS Eq. (1).

The dynamical formation of the condensate has been studied by means of self-similar solutions of the kinetic Eq. (2), leading to a finite time singularity for some time t_* [14,15]. This solution describes explicitly particle cumulation to zero wave number $\boldsymbol{k} = \boldsymbol{0}$. When the condensate begins to form ($t > t_*$), an exchange of mass between the condensate and the incoherent wave component is necessary to reach equilibrium. It was argued in Refs. [8,10,11] that this dynamics may be described by a kinetic three-wave interaction. More precisely, by extending the kinetic Eq. (2) to singular distributions $n_{\boldsymbol{k}}(t) = n_0(t)\delta^{(3)}(\boldsymbol{k}) + \phi_{\boldsymbol{k}}(t)$ [14,15], one gets a pair of coupled kinetic equations for the evolution of the condensate (n_0) and the incoherent wave component ($\phi_{\boldsymbol{k}}$) [15]. These equations describe a flux of mass from the incoherent component to the condensate, until equilibrium is reached, i.e., the collision terms vanish. This occurs for the equilibrium distribution

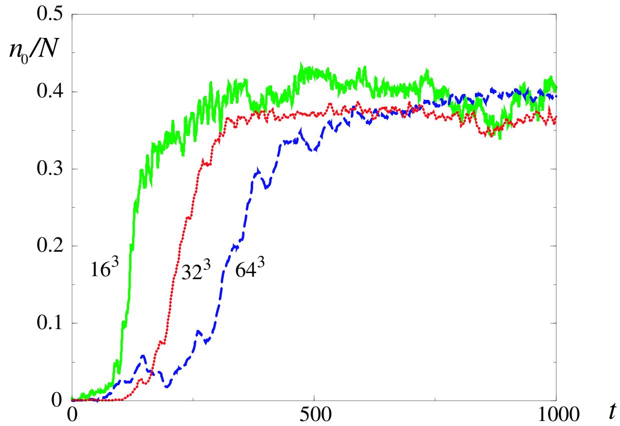

FIG. 1 (color online). Numerical simulations of the NLS Eq. (1) showing the temporal evolution of condensed particles n_0/N in 3D: independently of the number of computational modes, n_0/N tends to converge for long interaction times ($\langle H\rangle/V = 2$, $N/V = 1/2$, and $k_c = \pi/dx$ where $dx = 1$ refers to the spatial discretization of the NLS equation).

$\phi_k^{\mathrm{eq}} = T/k^2$, which actually corresponds to the distribution (3) with zero chemical potential. This allows us to legitimately assume $\mu = 0$ below the transition threshold $E \le E_{\mathrm{tr}}$. Note that $\mu = 0$ is also justified by the fact that the mass of the incoherent wave component is not conserved, due to its interaction with the condensate, which plays the role of a reservoir of particles.

The number of condensed particles n_0 and the energy E ($\le E_{\mathrm{tr}}$) may then be calculated by setting $\mu = 0$ in the equilibrium distribution (3). One readily obtains $(N - n_0)/V = 4\pi T k_c$ and $E/V = 4\pi T k_c^3/3$, which gives

$$n_0/N = 1 - E/E_{\mathrm{tr}}, \qquad (6)$$

or $n_0/N = 1 - T/T_{\mathrm{tr}}$, where $T_{\mathrm{tr}} = 3E_{\mathrm{tr}}/(4\pi V k_c^3)$. As in standard Bose-Einstein condensation, n_0 vanishes at the critical temperature T_{tr}, and n_0 becomes the total number of particles as T tends to zero. The linear behavior of n_0 vs E in Eq. (6) is consistent with the numerical simulations (see Fig. 2). However, note that Eq. (6) is derived for a spherically symmetric continuous distribution of $n_{\boldsymbol{k}}$, while the numerical integration is implicitly discretized. Equation (6) should thus be replaced by

$$\frac{n_0}{N} = 1 - \frac{E}{N}\frac{\sum_k{}' 1/(k_x^2 + k_y^2 + k_z^2)}{\sum_k{}' 1}, \qquad (7)$$

where $\sum_k{}'$ denotes a discrete sum for $-k_c \le k_x, k_y, k_z \le k_c$ that excludes the origin $k_x = k_y = k_z = 0$.

This distribution is plotted in Fig. 2 and compared with the numerical simulations of Eq. (1). The simulations started from a nonequilibrium distribution $\psi(\boldsymbol{x}, t = 0) = \sum_k a_{\boldsymbol{k}} \exp(i\boldsymbol{k}\cdot\boldsymbol{x})$, where the phases of the complex amplitudes $a_{\boldsymbol{k}}$ are distributed randomly [6–8]. They confirm the existence of the condensation process for sufficiently low energy densities [6]. We performed simulations with different numbers of computational modes (8^3, 16^3, 32^3, 64^3, and 128^3). Our numerical results reveal that once the number of modes exceeds 16^3, it only weakly affects the condensate fraction n_0/N (Fig. 1). This means that the system has reached some thermodynamic limit with only 16^3 modes.

The linear dependence (7) between n_0 and E gives a poor approximation of the numerical results, mainly because the condensate fraction has been calculated by taking into account only the linear (kinetic) contribution E to the total energy of the wave H. To include the nonlinear (interaction) contribution, we adapt the Bogoliubov expansion procedure of a weakly interacting Bose gas [16] to the classical wave problem considered here. Note that, within the dimensionless units adopted in Eq. (1), the standard criterion of applicability of Bogoliubov's theory [17] reads $(N/V)^{1/2}/(8\pi)^{3/2} \ll 1$. We start from the total energy H of the nonlinear wave $H = \sum_k k^2 a_{\boldsymbol{k}}^* a_{\boldsymbol{k}} + \frac{1}{2V}\sum_{k_1,k_2,k_3,k_4} a_{\boldsymbol{k}_1}^* \times a_{\boldsymbol{k}_2}^* a_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4}$, where $\delta_{\boldsymbol{k}}$ is the Kronecker delta symbol. The Hamiltonian may be decomposed into four terms, $H = H_0 + H_2 + H_3 + H_4$, depending on how the zero mode, $a_0 = a_{\boldsymbol{k}=\boldsymbol{0}}$, and nonzero modes, $a_{\boldsymbol{k}\neq 0}$, enter the expansion: $H_0 = \frac{1}{2V}[|a_0|^4 + 2|a_0|^2(N - |a_0|^2)]$, $H_2 = \sum_k{}'[(k^2 + \frac{|a_0|^2}{V})a_{\boldsymbol{k}}^* a_{\boldsymbol{k}} + \frac{1}{2V}(a_0^2 a_{\boldsymbol{k}}^* a_{-\boldsymbol{k}}^* + \mathrm{c.c})]$, $H_3 = \frac{1}{2V}\times \sum_{k_1,k_2,k_3}{}'(2a_0 a_{\boldsymbol{k}_1}^* a_{\boldsymbol{k}_2}^* a_{\boldsymbol{k}_3} + \mathrm{c.c.})\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3}$, $H_4 = \frac{1}{2V}\times \sum_{k_1,k_2,k_3,k_4}{}' a_{\boldsymbol{k}_1}^* a_{\boldsymbol{k}_2}^* a_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4} \times \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4}$, where $\sum_k{}'$ excludes the $\boldsymbol{k} = \boldsymbol{0}$ mode. The kinetic equation requires the Hamiltonian to be diagonal in quadratic terms. To this end, we apply the Bogoliubov's transformation for the canonical variables $b_{\boldsymbol{k}} = u_{\boldsymbol{k}} a_{\boldsymbol{k}} - v_{\boldsymbol{k}} a_{-\boldsymbol{k}}^*$, with the condition

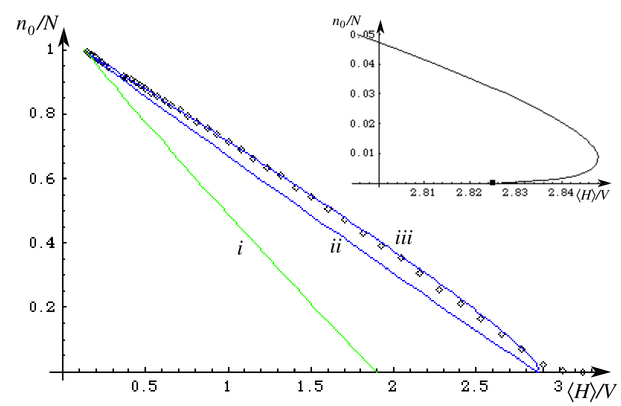

FIG. 2 (color online). Condensate fraction n_0/N vs total energy density $\langle H\rangle/V$, where $\langle H\rangle = E + E_0$, E_0 being the condensate energy [see Eq. (9)]. Points ($\Diamond$) refer to numerical simulations of the NLS Eq. (1) with 64^3 modes ($N/V = 1/2$). The straight line (i) [(ii)] corresponds to the continuous Eq. (6) [discretized Eq. (7)] approximation. Curve (iii) refers to condensation in the presence of nonlinear interactions [from Eq. (9)], which makes the transition to condensation subcritical, as illustrated in the inset (with 1024^3 modes). Each point ($\Diamond$) corresponds to an average over 10^3 time units.

$|u_k|^2 - |v_k|^2 = 1$ that preserves the Poisson's bracket relation $\{a_k, a_k^*\} = i$ in the b_k's basis. Imposing that the quadratic term H_2 is diagonal in this basis, we find $u_k = 1/\sqrt{1 - L_k^2}$ and $v_k = L_k/\sqrt{1 - L_k^2}$ with $L_k = [-k^2 - \rho_0 + \omega_B(k)]/\rho_0$ and $H_2 = \sum_k{}' \omega_B(k) b_k^* b_k$, where $\rho_0 = n_0/V \equiv |a_0|^2/V$, and $\omega_B(k) = \sqrt{k^4 + 2\rho_0 k^2}$ is the Bogoliubov's dispersion relation that takes into account the nonlinear interaction.

Let us emphasize that the kinetic equations describing the coupled evolution of the condensate (n_0) and the incoherent wave component (φ_k), are similar to those derived in Ref. [15], but the dispersion relation $\omega(k) = k^2$ is replaced by the Bogoliubov's expression $\omega_B(k)$. The equilibrium distribution turns out to be $\varphi_k^{\rm eq} = T/\omega_B(k)$, with $\langle b_k b_{k'}^* \rangle = \varphi_k^{\rm eq} \delta(\mathbf{k} - \mathbf{k}')$. In the b_k's basis, the uncondensed mass then reads

$$N - n_0 = \sum_k{}' \frac{k^2 + \rho_0}{\omega_B(k)} \varphi_k^{\rm eq} = T \sum_k{}' \frac{k^2 + \rho_0}{\omega_B^2(k)}. \quad (8)$$

The total averaged energy $\langle H \rangle$ has contributions from H_0, H_2, and H_4: $\langle H \rangle = E_0 + \sum_k{}' \omega_B(k) \varphi_k^{eq} = E_0 + T \sum_k{}' 1$, where $E_0 = \frac{1}{2V}[N^2 + (N - n_0)^2]$ is the energy of the condensate. The temperature T may be substituted from this expression by using Eq. (8), which gives a closed relation between $\langle H \rangle$ and n_0,

$$\langle H \rangle = E_0 + \frac{(N - n_0) \sum_k{}' 1}{\sum_k{}' [(k^2 + \rho_0)/\omega_B^2(k)]}. \quad (9)$$

This expression is in quantitative agreement with the numerical simulations of the NLS Eq. (1), without any adjustable parameter (see Fig. 2). Expression (9) remarkably reveals that the nonlinear interaction changes the nature of the transition to condensation, which becomes of the first order. This subcritical behavior is a small effect that has not been clearly identified in our numerical simulations.

In summary, by considering the defocusing NLS equation as a model, we showed that a classical nonlinear wave exhibits a subcritical condensation process in 3D, while no transition occurs in 2D. Numerical simulations of the NLS equation with stochastic initial conditions are found in quantitative agreement with the equilibrium distribution of the kinetic equation derived from the NLS equation. In spite of the formal reversibility of the NLS equation, the condensation process manifests itself through an irreversible evolution of the field towards a homogeneous plane wave (condensate) with small-scale fluctuations superimposed (uncondensed particles), which store the information necessary for time reversal. Our study is thus conceptually different from that reported in Ref. [9], in which the forced and dissipative (nonconservative) NLS equation is considered. We formulate a thermodynamic description of the condensation process, whose properties are analogous to those of standard Bose-Einstein condensation in quantum systems. However, caution should be exercised when drawing conclusions about condensation in real bosonic systems, because the NLS equation describes only highly occupied modes satisfying $n_k \gg 1$, so that it cannot describe any transfer of mass between scarcely occupied (high-energy) modes and the condensate [5–7,12,15].

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