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 condensation process by using a wave turbulence theory with ultraviolet cut-off. In 3 dimensions the equilibrium state undergoes a phase transition for sufficiently low energy density, while no transition occurs in 2 dimensions, in analogy with standard Bose-Einstein condensation in quantum systems. Numerical simulations show that the thermodynamic limit is reached for systems with 16^3 computational modes and greater. 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 simulations.

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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. Nevertheless, an important insight was obtained from *soliton* dynamics, in particular through numerical simulations performed for the focusing nonintegrable nonlinear Schrödinger (NLS) equation [1, 2]. These studies revealed that this system 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 plays the role of a "statistical attractor" for the system, while the small-scale fluctuations contain, in principle, all information necessary for time reversal. Importantly, the solitary-wave solution corresponds to the solution that minimizes the energy (Hamiltonian), so that the system tends to relax towards the state of lowest energy, while the small-scale fluctuations compensate for the difference between the total energy and that of the coherent structure [2].

It is only recently that a statistical description of this self-organization process has been elaborated [3, 4]. Remarkably it turns out that when the Hamiltonian system is constrained by an additional invariant (*e.g.,* the mass), the increase of entropy of small-scale turbulent fluctuations *requires* the formation of coherent structures to "store" the invariant [4], so that it is thermodynamically advantageous for the system to approach the ground state which minimizes the energy [2].

In the present work we consider 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 towards a homogenous plane-wave [8, 9], as described by the weak turbulence theory [10]. This evolution is consistent with the general rule discussed above [2–4], because the plane-wave solution realizes the minimum of the energy (Hamiltonian) in the defocus-

ing case. Accordingly, the NLS equation would exhibit a kind of condensation process, a feature that has been accurately confirmed only recently in the context of thermal Bose fields, where intensive numerical simulations of the NLS equation have been performed in $3D$ [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 whose thermodynamic properties are analogous to those of Bose-Einstein condensation in quantum systems, despite the fact that the considered wave system is completely *classical*. Our analysis is based on the kinetic theory of the NLS equation, in which we introduce a frequency cut-off to regularize the ultraviolet catastrophe inherent to ensembles of classical waves (Rayleigh-Jeans paradox). This allows us to clarify the essential role played by the number of modes in the dynamical formation of the condensate. Furthermore, 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 towards a state of equilibrium (maximum entropy) *without generating a coherent structure that minimizes the energy* (Hamiltonian), in contrast with the general rule commonly accepted [2–4, 8].

Given the universal character of the NLS equation in nonlinear wave systems, the reported 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, in relation to the recent proposal of condensation for photons [11]. Moreover, the formal reversibility of the condensation process could be demonstrated by means of an optical phase-conjugation experiment [12]. In addition to optics, wave condensation could be relevant for hydrodynamic surface waves [13], on the basis of the recent progress on measurements of Zakharov's spectra. Moreover, our work is

also relevant to the important issue of strong wave turbulence [14], where the emergence and persistence of large scale coherent structures in the midst of small scale fluctuations is a common feature of many turbulent fluids, plasmas and optical wave systems.

We consider the normalized defocusing NLS equation in D spatial dimensions for the complex function ψ[15]:

$$i\partial_t \psi = -\Delta\psi + |\psi|^2\psi \qquad (1)$$

where Δ stands for the Laplace operator in dimension D. 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 $H = \int \left(|\nabla\psi|^2 + \frac{1}{2}|\psi|^4\right) d^D x$.

We address the dynamical formation of the condensate starting from a non-equilibrium stochastic initial condition for the wave ψ, which we take to be of zero mean and statistically homogenous. In spite of the formal reversibility of the NLS Eq.(1), the nonlinear wave ψ may exhibit an *irreversible* evolution towards thermal equilibrium. The salient properties of this evolution may be described by weak-turbulence theory. This theory derives, within certain approximations [10], an irreversible kinetic equation for the averaged wave-spectrum, $\langle a_{\mathbf{k}_1} a^*_{\mathbf{k}_2} \rangle = n_{\mathbf{k}_1}\delta^{(D)}(\mathbf{k}_1 - \mathbf{k}_2)$, $a_{\mathbf{k}}$ being the Fourier transform of ψ defined by $a_{\mathbf{k}}(t) = \int \psi(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}} d^D x$

$$\partial_t n_{\mathbf{k}_1}(t) = \mathcal{C}oll[n_{\mathbf{k}_1}] \equiv \int d^D k_2 d^D k_3 d^D k_4 W_{k_1,k_2;k_3,k_4}$$
$$\times \ (n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_1} + n_{\mathbf{k}_3} n_{\mathbf{k}_4} n_{\mathbf{k}_2} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} - n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_4})(2)$$

with $W_{k_1,k_2;k_3,k_4} = \frac{4\pi}{(2\pi)^D}\delta^{(D)}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4)\,\delta^{(1)}(k_1^2 + k_2^2 - k_3^2 - k_4^2)$ [10]. As for the usual Boltzmann's equation, Eq.(2) conserves the mass $N = V \int n_{\mathbf{k}}(t) d^D k$, the kinetic energy $E = V \int k^2 n_{\mathbf{k}}(t) d^D k$ (being V the system volume for $D = 3$ and the surface for $D = 2$), and exhibits a H-theorem of entropy growth $d\mathcal{S}/dt \geq 0$, where $\mathcal{S}(t) = \int \ln(n_{\mathbf{k}}) d^D k$ is the non-equilibrium entropy. Accordingly, the kinetic equation (2) describes an irreversible evolution of the wave-spectrum towards the Rayleigh-Jeans *equilibrium* distribution [10]:

$$n_k^{eq} = \frac{T}{k^2 - \mu}, \qquad (3)$$

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

The distribution (3) realizes the maximum of the entropy $\mathcal{S}[n_{\mathbf{k}}]$ and vanishes exactly the collision term, $\mathcal{C}oll[n_k^{eq}] = 0$. 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 cut-off k_c, i.e., we assume $n_{\mathbf{k}}(t) = 0$ for $k > k_c$. Note

that this cut-off 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 [10].

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

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

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

These equations should be interpreted as follows. The initial non-equilibrium state of the field ψ is characterized by a mass N and an energy E. The wave spectrum then relaxes to the equilibrium distribution (3), whose temperature T and chemical potential μ are determined by Eqs.(4,5): a given pair (N, E) then determines a unique pair (T, μ). An inspection of Eq.(4) reveals that μ tends to 0, i.e. λ_c diverges to infinity, for a non-vanishing 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 the analysis of the energy per particle E/N. There exists a non-vanishing critical energy per particle $E_{\rm tr}/N = k_c^2/3$ such that $\mu = 0$. Dividing (5) by (4), one gets $(E - E_{\rm tr})/(Nk_c^2) = \pi\sqrt{-\mu}/(6k_c) + \mathcal{O}\left(-\mu/k_c^2\right)$. Decreasing the energy per particle effectively cools the system, and one reaches a finite threshold $E_{\rm tr}$, below which condensation occurs.

The same 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 results that condensation no longer take place in $2D$. We have confirmed this result by direct numerical simulations of the wave equation (1). In contrast to the $3D$ case where the field ψ generates a coherent plane-wave (condensate), in $2D$ ψ remains a stochastic field of zero mean, whose spectrum evolves towards the equilibrium distribution (3) with $\mu \neq 0$, *i.e.*, with a finite correlation length λ_c.

The dynamical formation of the condensate has been studied using self-similar solutions of the kinetic equation (2), leading to a finite time singularity for some time t_* [16, 17]. Although this singularity is naturally regularized in the NLS dynamics, it describes explicitly particle cumulation to zero wave-number $\mathbf{k} = 0$. 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, 9] that this dynamics may be described by a three-wave kinetic interaction (the fourth wave being the condensate). This aspect has been recently expressed more precisely by extending the kinetic equation (2) to singular distributions

$n_{\mathbf{k}}(t) = n_0(t)\delta^{(3)}(\mathbf{k}) + \phi_{\mathbf{k}}(t)$ [16, 17], so that a pair of coupled kinetic equations for the evolution of the condensate (n_0) and the incoherent wave-component ($\phi_{\mathbf{k}}$) has been derived [17]. These equations describe a flux of mass from the incoherent component towards the condensate, until thermal equilibrium is reached, i.e., until the collision terms exactly vanish. This occurs for the equilibrium distribution $\phi_k^{eq} = T/k^2$, which actually corresponds to the distribution (3) with zero chemical potential. This allows us to legitimately assume $\mu = 0$ below the transition threshold $E \leq E_{\mathrm{tr}}$.

The number of condensed particles n_0 and the energy $E(\leq E_{\mathrm{tr}})$ 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

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

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 0. The linear behavior of n_0 vs. E in Eq.(6) is consistent with the results of numerical simulations (see Fig. 1). However note that Eq.(6) is derived for a spherically symmetric continuous distribution of $n_{\mathbf{k}}$, while in the numerics the integration is discretized. Eq.(6) should thus be replaced by

$$\frac{n_0}{N} = 1 - \frac{E}{N}\frac{\sum'_k 1/(k_x^2 + k_y^2 + k_z^2)}{\sum'_k 1} \tag{7}$$

where $\sum'_k$ denotes a discrete sum for $-k_c \leq k_x, k_y, k_z \leq k_c$ that excludes the origin $k_x = k_y = k_z = 0$.

This distribution is plotted in Fig.1 and compared with that given by the numerical simulations of Eq.(1). In our simulations we started with a non-equilibrium distribution $\psi(\mathbf{x}, t = 0) = \sum_k a_k \exp(i\mathbf{k} \cdot \mathbf{x})$, where the phases of the complex amplitudes $a_{\mathbf{k}}$ are distributed randomly [6, 7]. The numerical simulations confirm the existence of the condensation process for sufficiently low energy densities [6]. We performed simulations with different number 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. This means that the system has reached some thermodynamic limit with only 16^3 modes. Moreover, we verified that for a given total volume V and a fixed density N/V, the energy threshold for condensation increases, as the frequency cut-off increases, in agreement with the theory ($E_{\mathrm{tr}} \propto k_c^2$).

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's theory of a weakly interacting Bose gas [18] to the classical wave problem considered here. We start from the
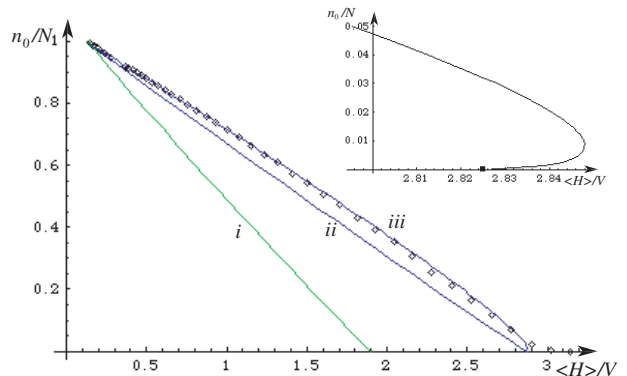

FIG. 1: Condensate fraction n_0/N vs. total energy density $\langle H \rangle / V$, where $\langle H \rangle = E + E_0$, E_0 being the condensate energy [see Eq.(9)]. Points ($\diamond$) refer to numerical simulations of the NLS Eq.(1) with 64^3 modes for a fixed density $N/V = 1$ ($k_c = \pi$). The 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).

total energy H of the nonlinear wave

$$H = \sum_k k^2 a_{\mathbf{k}}^* a_{\mathbf{k}} + \frac{1}{2V}\sum_{k_1,k_2,k_3,k_4} a_{\mathbf{k_1}}^* a_{\mathbf{k_2}}^* a_{\mathbf{k_3}} a_{\mathbf{k_4}} \delta_{\mathbf{k_1}+\mathbf{k_2}-\mathbf{k_3}-\mathbf{k_4}},$$

where $\delta_{\mathbf{k}}$ 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, $a_0 = a_{\mathbf{k}=0}$, and non-zero modes, $a_{\mathbf{k}\neq0}$, enter the expansion:

$$H_0 = \frac{1}{2V}\left(|a_0|^4 + 2|a_0|^2(N - |a_0|^2)\right)$$

$$H_2 = \sum_k' \left[\left(k^2 + \frac{|a_0|^2}{V}\right)a_{\mathbf{k}}^* a_{\mathbf{k}} + \frac{1}{2V}\left(a_0^2 a_{\mathbf{k}}^* a_{-\mathbf{k}}^* + c.c\right)\right]$$

$$H_3 = \frac{1}{2V}\sum_{k_1,k_2,k_3}' (2a_0 a_{\mathbf{k_1}}^* a_{\mathbf{k_2}}^* a_{\mathbf{k_3}} + c.c.)\delta_{\mathbf{k_1}+\mathbf{k_2}-\mathbf{k_3}}$$

$$H_4 = \frac{1}{2V}\sum_{k_1,k_2,k_3,k_4}' a_{\mathbf{k_1}}^* a_{\mathbf{k_2}}^* a_{\mathbf{k_3}} a_{\mathbf{k_4}} \delta_{\mathbf{k_1}+\mathbf{k_2}-\mathbf{k_3}-\mathbf{k_4}},$$

where $\sum_k'$ excludes the $\mathbf{k} = 0$ 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 $b_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a_{-\mathbf{k}}^*$, with the condition $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$ that preserves the Poisson's bracket relation $\{a_{\mathbf{k}}, a_{\mathbf{k}}^*\} = i$ in the $b_{\mathbf{k}}$'s basis. Imposing that the quadratic term H_2 is diagonal in this basis, we find $u_{\mathbf{k}} = 1/\sqrt{1 - L_{\mathbf{k}}^2}$ and $v_{\mathbf{k}} = L_{\mathbf{k}}/\sqrt{1 - L_{\mathbf{k}}^2}$ with $L_{\mathbf{k}} = [-k^2 - 2\rho_0 + \omega_B(k)]/\rho_0$ and $H_2 = \sum_k' \omega_B(k) b_{\mathbf{k}}^* b_{\mathbf{k}}$, 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, in the $b_\mathbf{k}$'s basis, the kinetic equations describing the coupled evolution of the condensate (n_0) and the incoherent wave-component ($\varphi_\mathbf{k}$), are similar to those derived in Ref.[17], but the linear dispersion relation $\omega(k) = k^2$ is replaced by the Bogoliubov's expression $\omega_B(k)$. The equilibrium distribution turns out to be $\varphi_k^{eq} = T/\omega_B(k)$, with $\langle b_\mathbf{k} b_{\mathbf{k}'}^* \rangle = \varphi_k^{eq}\delta(\mathbf{k}-\mathbf{k}')$, so that the uncondensed mass (in the $b_\mathbf{k}$'s basis) reads

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

The total averaged energy $\langle H \rangle$ has contributions from H_0, H_2 and H_4 [19]: $\langle H \rangle = E_0 + \sum_k' \omega_B(k)\varphi_k^{eq} = E_0 + T\sum_k' 1$, where $E_0 = \frac{1}{2V}\left[N^2 + (N-n_0)^2\right]$ 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,

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

This expression is in quantitative agreement with the numerical simulations of the NLS Eq.(1), without any adjustable parameter (see Fig. 1). 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 more pronounced when the number of modes increases.

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 $2D$. In spite of the formal reversibility of the NLS equation, the condensation process manifests itself by means of an irreversible evolution towards a homogenous plane-wave (condensate), with small-scale fluctuations superimposed (uncondensed particles), which store the information necessary for time reversal. 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 only describes highly occupied modes satisfying $n_\mathbf{k} \gg 1$, so that it cannot describe any transfer of mass between scarcely occupied high-energy modes and the condensate [5–7, 17]. Such a transfer is crucial at least at the beginning of the growth of the condensate that starts with zero mass.

To conclude we would like to mention that the equilibrium distribution (3) also describes the velocity spectrum distribution in $2D$ fluid turbulence [20]. An analogy between $2D$ fluid turbulence and our results may be helpful in the context of decaying turbulence at very high Reynolds number [21]. In this case, following Onsager's argument [22], the large scale vortices formed by the inverse cascade would play the role of the condensate.

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[19] The H_4 term is not of higher order than H_0 or H_2. After a rapid inspection, one sees that particular terms where all four k_α's ($\alpha = 1, 2, 3, 4$) are the same, or those where: $k_1 = k_3$, $k_2 = k_4$ (and $3 \leftrightarrow 4$) contribute up to a first order. Other terms introduce correlations which are treated through the random phase approximation. The final sum in H_4 reads $H_4 = \frac{1}{2V}\left(\sum_\alpha' |a_\alpha|^4 + 2\left(\sum_\alpha' |a_\alpha|^2\right)\left(\sum_\beta' |a_\beta|^2\right)\right)$. How-

ever, the $\sum'_\alpha |a_\alpha|^4$ is definitively negligible.

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