Condensation of Classical Nonlinear Waves in a Two-Component System

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We study the formation of large-scale coherent structures (a condensate) for a system of two weakly interacting classical waves. Using the coupled defocusing nonlinear Schrödinger (NLS) equations as a representative model, we focus on condensation in the phase mixing regime. We employ weak turbulence theory to provide a complete thermodynamic description of the classical condensation process. We show that the temperature and the condensate mass fractions are fully determined by the total number of particles in each component and the initial total energy. Moreover, we find that, at higher energies, condensation can occur in only one component. The theory presented provides excellent agreement with results of numerical simulations obtained by directly integrating the dynamical model.

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Many classical systems in nature reveal the emergence of large-scale coherent structures from a background of irregular field characterised by small-scale fluctuations. Examples of systems that exhibit such behavior include classical turbulence, nonlinear optics, superfluids, ultracold gases and Bose-Einstein Condensates (BECs), and the formation of the early universe. In certain regions of the parameter space, a large sub-class of these systems can be described by a system of weakly nonlinear dispersive waves. A universal equation that governs the evolving field in such scenarios is then given by the Nonlinear Schrödinger (NLS) equation. The process of self-organisation in the focusing NLS equation has been studied in [1]. It was found that a large-scale solitary wave tends to emerge from a sea of small-scale turbulent fluctuations. In this work, we concentrate on the defocusing NLS equation. This equation has been receiving increasing attention due to the experimental advances in BECs. In this context, the defocusing NLS equation corresponds to the Gross-Pitaevskii (GP) equation [2] of a homogeneous Bose gas. The GP equation has long been used as a model of a weakly interacting Bose gas at zero temperature. More recently, it has been argued [3] that the GP equation can be used to model the long wavelength part of the spectrum of a BEC at finite temperatures. Numerical simulations conducted within this framework [4, 5] have indeed confirmed this, revealing the ability of the model to capture the formation of a condensate from an initially turbulent state.

With the rapid developments being made in experimental techniques, it is now possible to realize multicomponent BECs formed by the simultaneous trapping and cooling of atoms in distinct spin or hyperfine levels [6] or different atomic species [7]. The finite temperature dynamics of such Bose gas mixtures is then governed by a system of coupled NLS equations. While such systems are of interest in their own right, they also serve as idealised models to study symmetry-breaking phase transitions that are believed to have occurred in the early evolution of the universe. A specific example is given by the Kibble-Zurek mechanism [8] of the formation of topological defects following the rapid quench of the system below the point of second-order phase transitions. This scenario would correspond to the formation of cosmological vortons and springs that are analogous to the vortex ring-slab and vortex ring-vortex ring complexes of BECs [9]. In addition to these physical examples, the coupled NLS equations are also encountered in the study of optical fibres and electromagnetic waves [10]. Given the universality of these equations in the nonlinear sciences, an accurate thermodynamic description of the condensation process in such a system could have significant implications in various branches of physics.

In this Letter, we will generalise the results presented in [11], that describe the condensation process of a one-component system, to a two-component system. We note that two-component systems tend to show a broad class of qualitatively different behavior depending on the relative strengths of the intercomponent and intracomponent interactions. This can lead to contrasting regimes of condensation: the phase mixing regime and the phase separation regime [12]. Consistent with our original assumptions of weakly interacting systems, we will focus exclusively on the phase mixing regime.

We begin by considering the scenario of a system of two weakly interacting classical waves (e.g. Bose gases consisting of the same atoms in different spins) that have been rapidly cooled below the transition temperature. Their evolution from the resulting strongly nonequilibrium initial state is then described by the coupled NLS equations given by

\[ i \partial_t \psi_1 = -\nabla^2 \psi_1 + |\psi_1|^2 \psi_1 + \alpha |\psi_2|^2 \psi_1, \]
\[ i \partial_t \psi_2 = -\nabla^2 \psi_2 + |\psi_2|^2 \psi_2 + \alpha |\psi_1|^2 \psi_2, \]  

where \( \psi_1 \) and \( \psi_2 \) are complex-valued classical fields corresponding to each component, and \( \alpha \) is the intracompo-
nent coupling constant. For the phase mixing regime, we require \( 0 < \alpha < 1 \). The dynamics governed by the above equations will conserve the total mass (number of particles) given by \( N_1 = \int |\psi_1|^2 d\mathbf{x} \) and \( N_2 = \int |\psi_2|^2 d\mathbf{x} \). In addition, the total energy (Hamiltonian) of the coupled system

\[
H = \int \left[ \sum_{i=1}^{2} \left( \frac{1}{2} (\nabla \psi_i)^2 + \frac{\alpha}{2} |\psi_1|^2 |\psi_2|^2 \right) + \frac{1}{2} |\psi_1|^2 |\psi_2|^2 \right] dV. \tag{2}
\]

will be conserved. Without loss of generality we shall assume that \( N_2 \leq N_1 \).

Despite the formal reversibility of the above Hamiltonian system, the evolution of the nonlinear waves \( \psi_1 \) and \( \psi_2 \) is not integrable giving rise to an effective diffusion in phase space. This results in an irreversible evolution to thermal equilibrium. By invoking the random phase approximation (assumption of quasi-Gaussian statistics), it is possible to derive closed irreversible kinetic equations that describe the evolution of the system using Weak Turbulence Theory (WTT) \cite{13}. For a homogeneous system, we accomplish this by expressing the order parameters in terms of their Fourier transforms

\[
\psi_1 = \frac{1}{(2\pi)^{d/2}} \int \hat{a}_k(t) e^{ik \cdot \mathbf{x}} d\mathbf{k}, \quad \psi_2 = \frac{1}{(2\pi)^{d/2}} \int \hat{b}_k(t) e^{ik \cdot \mathbf{x}} d\mathbf{k}.
\]

Substituting into Eq. (4), we can derive expressions from the spectral number densities \( \langle \hat{a}_k, \hat{a}_k^* \rangle = n_1 \delta(\mathbf{k_1} - \mathbf{k}_2); \langle \hat{b}_k, \hat{b}_k^* \rangle = \lambda_1 \delta(\mathbf{k_1} - \mathbf{k}_2) \). Provided the nonlinearity in the system is sufficiently weak (i.e. \( N_1/V \ll 1; N_2/V \ll 1; \alpha \ll 1 \), where \( V \) is the volume of the system), we can derive the kinetic equation

\[
\partial_t n_k = \frac{4\pi}{(2\pi)^d} \int \left[ \left( (n_k + 1)n_2 n_3 - n_k n_1 (n_2 + n_3) \right) + \alpha^2 \left( (n_k + 1)l_2 n_3 - n_k l_1 (l_2 + n_3) \right) \right]
\]

\[
\times \delta(k + k_1 - k_2 - k_3) \delta(k^2 + k_1^2 - k_2^2 - k_3^2) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3. \tag{3}
\]

Similarly, an equation for \( l_k \) can be derived and followed directly from above by the symmetry in Eq. (1). These equations conserve \( N_1 = V \int n_k(t)d\mathbf{k}, \quad N_2 = V \int l_k(t)d\mathbf{k} \), and the kinetic energies \( E_1 = V \int k^2 n_k(t)d\mathbf{k}, \quad E_2 = V \int k^2 l_k(t)d\mathbf{k} \) for each component. They admit two formal equilibrium solutions; the first corresponding to a uniform distribution \( n_k^{eq} = c_1, l_k^{eq} = c_2 \), and the second given by the Rayleigh-Jeans (RJ) distribution

\[
n_k^{eq} = \frac{T}{k^2 - \mu_1}, \quad l_k^{eq} = \frac{T}{k^2 - \mu_2}. \tag{4}
\]

Here, \( T \) is the thermodynamic temperature, and \( \mu_1 \) and \( \mu_2 \) are the chemical potentials. Equation (4) satisfies a H-theorem for entropy growth which implies that the RJ distribution will be realized in practice. However, Eq. (4) provides only a formal solution since it leads to non-convergent expressions for \( N_1, N_2 \), and the kinetic energies \( E_1, E_2 \) as \( k \to \infty \). We recall that, for BECs, Eq. (1)

is valid in the limit of large occupation numbers where a semi-classical description is valid. When \( n_k \approx 1 \) and \( l_k \approx 1 \), Eq. (1) begins to break down and a full quantum mechanical treatment of the problem becomes necessary. To regularise the ultra-violet catastrophe, we introduce a cut-off \( k_c \) such that \( n_k^2(|k_c|) \gg 1, l_k^2(|k_c|) \gg 1 \). This cut-off does not affect the equilibrium state provided a sufficiently large number of modes can be represented classically \cite{3, 14}. The reason is that a full quantum mechanical description corresponds to a grand-canonical ensemble with fluctuations in particle number and energy. However, for sufficiently many modes, such fluctuations will be small and we can introduce the above truncation to reduce the system to a microcanonical ensemble where the number of particles and the energy are conserved.

The RJ distributions corresponding to Eq. (3) are only valid at sufficiently high energies when no condensate is present. At sufficiently low energies, Eq. (3) breaks down very rapidly giving way to the formation of a condensate as elucidated in numerical simulations for a one-component system \cite{3, 3, 11} and a two-component system \cite{13}. In the simplest scenario, condensates with zero wavenumbers are formed and are associated with the uniform states provided we are in the phase mixing regime. If the condensates that form are strong in the sense that \( (N_1 - n_o)/N_1 \ll 1, (N_2 - l_o)/N_2 \ll 1 (n_o = |a_o|^2; l_o = |b_o|^2) \) are the occupation numbers of the condensates in components 1 and 2, respectively, one can describe the nonlinear dynamics at these later times by considering the evolution of small quasiparticle perturbations around the condensates. For our two-component system, we accomplish this by introducing the ansatz \( a_k = [\sqrt{n_o} \delta(k) + \bar{a}_k(t)] e^{-i\omega_n t}, \quad b_k = [\sqrt{l_o} \delta(k) + \bar{b}_k(t)] e^{-i\omega_n t} \). Upon substituting these expressions into the Fourier-transform representation of Eq. (2), we introduce a transformation to diagonalize terms in the Hamiltonian that are quadratic in \( \bar{a}_k \) and \( \bar{b}_k \). A generalisation of Bogoliubov's transformation \cite{13} to diagonalise the Hamiltonian in two-component systems was given in \cite{17}. To this end, we introduce the canonical variables \( \mathcal{N} = (\xi_k, \eta_k)^T \) which are related to the original variables \( \mathcal{A} = (\bar{a}_k, \bar{b}_k)^T \) through the relation

\[
\begin{pmatrix} \mathcal{A} \\ \mathcal{A}^\dagger \end{pmatrix} = \begin{pmatrix} U^+ & U^- \\ U^+ & U^- \end{pmatrix} \begin{pmatrix} \mathcal{N} \\ \mathcal{N}^\dagger \end{pmatrix}, \tag{5}
\]

where \( \mathcal{N}^\dagger = (\xi^*_k, \eta^*_k)^T \), and \( \mathcal{A} = (\bar{a}^*_k, \bar{b}^*_k)^T \). To preserve the properties of the Poisson bracket in the new basis, the transformation must satisfy the condition \( U^+ U^- - U^- U^+ = I \). A transformation that satisfies this condition and diagonalises the quadratic term is obtained when the elements \( u_{ij}^\pm \) of the \( 2 \times 2 \) transformation matrices \( U^\pm \) are given by

\[
U^\pm = \begin{pmatrix} \Gamma_{1,1}^\pm & \pm \Gamma_{1,2}^\pm \\ \Gamma_{2,1}^\pm & \pm \Gamma_{2,2}^\pm \end{pmatrix} \begin{pmatrix} \cos \gamma_k & \pm \sin \gamma_k \\ \pm \sin \gamma_k & \pm \cos \gamma_k \end{pmatrix}. \tag{6}
\]
\[ \Gamma^2 \frac{\partial}{\partial \mathbf{k}} = \sqrt{k^2 + \Omega^2} \] denotes the ratios of the dispersion relations, where \( \Omega^\pm = \sqrt{k^2 + c^2 \pm 2k} \) and \( c^{\pm} = |a_o + l_o \pm \sqrt{(n_o - l_o)^2 + 4n_o^2l_o}/V; \) sin \( \gamma_k = \left( \frac{1}{2} \left[ 1 - \frac{1 - r}{\sqrt{(1 - r)^2 + 4z^2}} \right] \right) \cdot \cos \gamma_k = \left( \frac{1}{2} \left[ 1 + \frac{1 - r}{\sqrt{(1 - r)^2 + 4z^2}} \right] \right), \]

where \( r = l_o/n_o \) and \( z = \alpha \sqrt{l_o/n_o} \). The resulting expression for the Hamiltonian leads to kinetic equations for the canonical (quasiparticle) densities \( \langle \tilde{n}_k, \tilde{c}_k \rangle = \tilde{n}_1 \delta(k_1 - k_2); \langle \tilde{n}_k, \tilde{c}_k \rangle = \tilde{n}_1 \delta(k_1 - k_2) \) which are given by

\[ \partial_t \tilde{n}_k = \pi \left( [R_{k12} - R_{k21} - k_{12}k_{21}] + [S_{k12} + S_{k21}] + [T_{k12} - T_{k21} + U_{k12} + V_{k12}] \right) \]

\[ \frac{1}{2} \sum_{k} [\langle \tilde{n}_k \rangle^2 - \tilde{n}_k \tilde{n}_k - \tilde{n}_k \tilde{n}_k] \delta(\Omega^+ - \Omega^-), \]

\[ S_{k12} = \left( \frac{\tilde{n}_1 \tilde{n}_k}{2} - \tilde{n}_1 \tilde{n}_k \tilde{z} \right)^2 \delta(\Omega^+ - \Omega^-), \]

\[ T_{k12} = \left( \tilde{n}_1 \tilde{n}_k \tilde{z} \right)^2 \delta(\Omega^+ - \Omega^-), \]

\[ U_{k12} = \left( \tilde{n}_1 \tilde{n}_k \tilde{z} \right)^2 \delta(\Omega^+ - \Omega^-), \]

\[ V_{k12} = \left( \tilde{n}_1 \tilde{n}_k \tilde{z} \right)^2 \delta(\Omega^+ - \Omega^-), \]

where \( \Delta^{(i)} \) denotes coefficients that will, in general, depend on \( \tilde{u}_{ij}^\pm, n_o, l_o \) and \( \alpha \). Since we are only interested in equilibrium solutions, their precise form is not too important. The equation for \( h_k \) follows by symmetry of the dynamical equation. These kinetic equations are now given by resonant three-wave interactions and have a parameterized family of solutions given by \( \tilde{n}_k = T/\Omega^+ (k) \), and \( \tilde{c}_k = T/\Omega^- (k) \), respectively. The condensates, therefore, strongly affect the equilibrium distributions of the quasiparticles.

Using these equilibrium solutions, we can now derive a relation between the occupation numbers \( n_o, l_o \), and the total number of particles \( N_1, N_2 \) and the energy \( H \). For a finite sized system, the Hamiltonian can be expressed in terms of the Fourier series \( \psi_1 = \sqrt{\frac{V}{\Omega}} \sum_{k} a_k \exp(\mathbf{ik} \cdot \mathbf{x}) \), \( \psi_2 = \sqrt{\frac{V}{\Omega}} \sum_{k} b_k \exp(\mathbf{ik} \cdot \mathbf{x}) \). The Hamiltonian can then be written as \( H = H_o + H_2 + H_3 + H_4 \) depending on how \( a_o = a_k = 0 \) and \( b_o = b_k = 0 \), and non-zero modes enter the expansion:

\[ H_o = \frac{1}{2} \sum_{k} \left( \left(a_o^2 + a_k^2 + b_o^2 + b_k^2\right) \left(N_1 - a_o^2 + b_o^2 + 2b_k^2\right) \right) + \frac{1}{2} \left( \left[a_o^2 + b_o^2 + N_2^2\right] \right), \]

\[ H_2 = \sum_{k} \left( \sum_{i} \left| k_i^2 \right| \right) a_k a_k^* \right) + 
\]
and now $E_0 = \frac{1}{\Omega} [N_1^2 + (N_1 - n_o)^2 + 2N_2^2 + 2\alpha N_1 N_2]$. This equation provides two algebraic expressions for the two unknowns $n_o$ and $\mu_2$. We note that at the critical energy where the condensate in the second component vanishes, we have $l_o = 0$ and $\mu_2 = 0$. At this point, it can be shown that the equilibrium distributions given by $\frac{T}{\mu_2}$ and $\frac{T}{\mu_1}$ reduce to $\frac{T}{\mu_2}$ and $\frac{T}{\mu_1}$ and the two solutions given above match at the critical energy. This provides a solution for the thermodynamic state that is uniformly valid over the entire range of energies.

To verify the theory, we numerically solved the coupled system in a cubic region with periodic boundary conditions using a pseudo-spectral method with spatial resolution containing $(64)^3$ grid points and a time-step of 0.01. The initial conditions were set using the random phase approximation (see e.g. [4]). To determine the properties of the system at equilibrium, we assumed that the ergodic hypothesis applies and used time-averages from our simulations to represent ensemble averages that arise in the theory presented above. Figure 1 presents results for the variation of the condensate mass fractions with $\langle H \rangle$. The results shown reveal remarkable agreement with the theory presented over the entire range of energies. For very large energies where only a small condensate mass fraction of the first component is present, the theory deviates very slightly from the results of the simulations. This occurs since many particles are non-condensed in this region violating the assumption of a strong condensate that is required for the theory.

Given the excellent agreement between the theory and predictions, we can use Eq. (11) to determine how the critical energy ($\langle H \rangle_{\text{crit}}$), at which condensation in the second component ceases, varies with the discrepancy parameter $\sigma = \frac{N_1 - n_1}{N_2}$. The variation of $\langle H \rangle_{\text{crit}}$, nondimensionalised with respect to the value at $\sigma = 0$ ($\langle H \rangle_{\text{ref}}$), is shown in the inset of Fig. 1. The figure clearly illustrates that $\langle H \rangle_{\text{crit}}$ deviates significantly from its value at $\sigma = 0$ as the discrepancy parameter is increased giving rise to a range of energies where only the first component condenses.

In summary, we have derived a theoretical formulation of the thermodynamic state governed by the coupled NLS equations for a classical system of two weakly interacting waves in 3D. Numerical simulations are in excellent quantitative agreement with the theory that is based on the equilibrium solutions of the kinetic equations for the NLS system of equations. The study presented here is relevant in quantifying condensation in a number of physical systems. Notable examples include mixtures of BEC gases at finite temperature and nonlinear optics provided many modes are present that can be modeled semi-classically.

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