Coalescence and Droplets in the Subcritical Nonlinear Schrödinger Equation

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We describe here the coalescence and formation of droplets, in a Hamiltonian kinetics of a first order phase transition. In the process of coalescence, the typical linear size of single phase domains grows as a power of time. The density correlation function follows the usual self-similar dynamic scaling. For different initial conditions, we observe the nucleation and dynamics of stable pulses. The stability of such pulses in one dimension is also computed. Both results may be relevant to superfluid He_4 cavitation or for filamentation in nonlinear optics and for the recent evidence of Bose-Einstein condensation in Li_7. [S0031-9007(97)02409-5]

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The well known process of the formation of singularities at finite time in nonlinear wave phenomena (for instance optics) is generically described by the (focusing) nonlinear Schrödinger equation [1]

$$i\partial_t\psi = \nabla^2\psi + |\psi|^2\psi\,. \tag{1}$$

Here ψ is a complex quantity representing the amplitude of the wave, i.e., the electric field in optics. The nonlinear term represents the action of a refraction index depending on the field intensity. For spatial dimensions equal and higher than two and for a large set of initial conditions the electric field diverges at a finite time.

Experimentally we observe in optics only a kind of filamentation, i.e., two dimensional pulses of very high but finite intensity (see, for instance, [2]). We may imagine that physically the appearance of singularities at finite time and collapsing waves are, in some sense, "fictions," since for very large electric fields we must include higher orders in the expansion of the nonlinear refraction index. As a consequence, the divergence is stopped, creating stable and intense light pulses. In He_4 superfluidity, those pulses must be regarded as superfluid droplets.

We study the formation of these localized structures when higher order terms are added to Eq. (1). We describe a Hamiltonian system where the energy has two local stable minima. In some sense, by analogy with the bifurcation theory, this can be called a "subcritical" conservative dynamic. The physics observed in the numerics is very analogous to the formation of droplets in a "dynamical" first order phase transition. By dynamical we mean that all the physical processes take place out of equilibrium; moreover, there is no explicit relaxation process: The dynamics are completely reversible (and Hamiltonian).

A purely variational (and nonconservative in the sense of matter) dynamics does not lead to stable droplets because of the minimization of the free energy of the system, which finally is completely filled by the most stable phase. However, stable solitary waves induced by subcritical nonvariational instabilities were discovered some time ago by Thual and Fauve [5] and studied in detail later [6]. In this case, the nonvariational effects stabilize the solitons.

In this Letter we show that stable solitary waves arise 1D, 2D, and 3D whenever we add a fifth power term to Eq. (1). We show also a mechanism of coalescence between the liquid droplets or gaseous bubbles, leading finally to two stable domains in a finite volume. This process follows a self-similar dynamical scaling. Finally, we argue that the pulses or droplets are stable because of the mechanism of coalescence which transfer (irreversibly) the matter of small droplets (perturbations) to the main drop, in a kind of condensation.

Our starting point is a subcritical nonlinear Schrödinger (SNLS) equation (we use the same notations as in [7] and in general we shall speak in the context of Bose superfluid at $T = 0$ K, that is, a liquid, instead of nonlinear optics)

$$i\frac{\partial\psi}{\partial t} = -\tfrac{1}{2}\nabla^2\psi - 2\rho_c|\psi|^2\psi + |\psi|^4\psi\,; \tag{2}$$

ρ_c is a constant. In general the inverse of ρ_c represents the small expansion parameter of the nonlinear terms: For $|\psi|^2 \ll \rho_c$ the cubic term [Eq. (1)] is sufficient to describe the phenomena; however, when $|\psi|^2 \approx \rho_c$, one must add the quintic term. Physically, for superfluid He II, ρ_c is related to the critical density for cavitation; that is, when the sound speed vanishes (see later), experimentally this happens for densities of the order of 0.1 $\mathrm{g/cm^3}$ [3]. In optics, the expansion parameter represents an electric field intensity being a characteristic of the material. Typically $\rho_c \approx 10^{22}\ \mathrm{V^2/m^2}$ (the characteristic intensity in atomic scales).

In a similar way, Eq. (2) could be a good model to study the dynamics of the many body system of attractive two particles interaction which is the case of Li_7 [4]. If one neglects the three body interactions, this ultracold gas is unstable as in the case of nonlinear optics; however, it was suggested (see Ref. [13] of [4]) that the external magnetic forces, used to trap the atoms, could stop the collapse, in an unclear way because the magnetic field varies so slowly in the small region of the collapse. The three particle interaction has to be repulsive in order to regularize singularities; thus our results could be relevant in the recent experiments of Bose-Einstein condensation of Li_7.

Equation (2) possesses the following invariances: (i) translation, (ii) Galilean invariance, and (iii) global phase change. The total mass or number of particles, $N = \int |\psi|^2 d^D x$, is conserved, as well as the energy:

$$H = \int (\tfrac{1}{2}|\nabla\psi|^2 - \rho_c|\psi|^4 + \tfrac{1}{3}|\psi|^6) d^D x \,. \qquad (3)$$

The long wavelength behavior of the system is described by a phase variable, the phase of ψ, which follows a wave equation. The variations of the modulus of ψ are related to the phase fluctuations. It is useful to define $\rho = |\psi|^2$ which we shall call the local "density of the liquid" ("light intensity" in nonlinear optics). The density ρ satisfies a wave equation: $\partial_{tt}\rho = c^2\nabla^2\rho$, c being the sound velocity. For a density ρ the sound speed is $c = \sqrt{2\rho(\rho - \rho_c)}$; therefore, it vanishes for $\rho = \rho_c$. If the local density ρ is less than ρ_c, a long wavelength instability develops because locally c^2 becomes negative. The linear density perturbation $\rho + \delta\rho_k e^{ik\cdot x + \sigma_k t}$, with $\sigma_k = \sqrt{k_0^2 k^2/2 - k^4/4}$ and $k_0^2 = 4\rho(\rho_c - \rho)$, are unstable for all perturbations such that $k < \sqrt{2}k_0$. Starting with an initial uniform density ρ_0 slightly less than ρ_c, the density variations grow exponentially in time, as one can see in Fig. 2(a), creating a cellular modulation with the length scale of the fastest growing mode, i.e., $1/k_0$; see Fig. 1(a). This very short scale modulation expels matter from one domain to another, creating regions with more stable densities, and leading to a splitting of space into well defined domains with large ($\sim\rho_c$) and small (~ 0) stable densities.

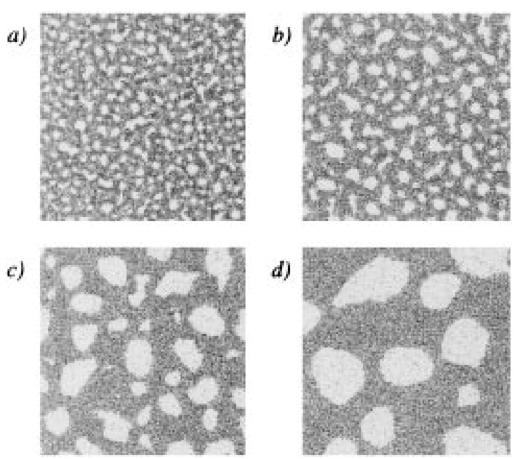

FIG. 1. A time sequence of the coalescence of gas bubbles. The gray scale represents the vapor phase by a light gray and the liquid by a dark gray. The images are taken (a) at $t = 36.2$, (b) $t = 61.1$, (c) $t = 203.35$ and (d) $t = 634.7$ time units. The number of bubbles decreases in time following the law $n \sim t^{-1}$, as usual in coalescence phenomena. We used a Gauss-Seidel Crank-Nicholson finite-difference method in a $(256)^2$ box with Neuman boundary conditions, $dx = 1.0$, $\rho_c = 1.1$, and $\rho_0 = 1$.

A second intermediary and short stage in the process occurs: The pressure difference between the low density (gas) and the large density (liquid) phases contract the liquid phase, until the liquid density reaches $\frac{3}{2}\rho_c$, the point where pressure equilibrium is established. Finally, one can observe a third step, with slow spatiotemporal dynamics, where the stable droplets and bubbles coalesce: The number of domains diminishes inversely proportional to the time. This process may be seen by the simple kinetic process $B + B \to B$. Let $n(t)$ be the total number of bubbles B by volume unit; then, if we suppose the diffusion constant independent of the radius of the bubble, the number of bubbles follows the rate equation [8]

$$\frac{dn}{dt} \sim -n^2,$$

i.e., $n \sim t^{-1}$ as we observe in the numerical simulations in two and three spatial dimensions (see Figs. 1 and 2); however, in 1D the number of domains decreases only as $n \sim t^{-1/4}$, lacking a satisfactory explanation.

Indeed, we observe that the typical size of structures grows as $\ell(t) \sim t^{1/2}$ in two spatial dimensions and $\ell(t) \sim t^{1/3}$ in three spatial dimensions [$\ell(t) \sim t^{1/4}$ in 1D] as shown in Fig. 2(b); moreover, numerical simulations show that the structure factor $S(k,t) = \langle|\psi_k(t)|^2\rangle$ [$\psi_k(t)$ being the Fourier transform of $\psi(x,t)$ and $\langle\cdots\rangle$ the angular average in Fourier space] evolves as

$$S(k,t) = \ell(t)^D S(\ell(t)k) \,,$$

where $S(\cdot)$ is a universal function for large t [9]. Figure 2 plots the function $S(k,t)/\ell(t)^D$ as a function of $\ell(t)k$ for different times in 2D. One can see the convergence to the universal function S for large t, as well as the exponential growth of $S(k,t)$ at a defined scale for small t. In addition, let us notice that S follows the Porod law, i.e., $S(u) \sim u^{-(D+1)}$, at least in 2D, which means that we are dealing with sharp domain walls [9].

This kind of physical process is not the only one possible; it happens for an initial condition such that the initial ratio ρ_0 is close from ρ_c, which is the case of superfluid helium. However, in nonlinear optics the electric field amplitude is usually much less than an atomic one; thus $\rho_0 \ll \rho_c$. This is also the case of condensates of Li_7 since the total number of trapped atoms is very small. In both cases, the fifth power term is negligible in (2) and the focusing instability tends naturally towards singular points in a finite time, until the amplitude of $|\psi|^2$ becomes comparable with ρ_c, at which point the fifth power term "saturates" the focusing instability and leads to the formation of stable droplets as seen in Fig. 3 for a 2D simulation. This kind of situation seems to be the one observed in nonlinear optics.

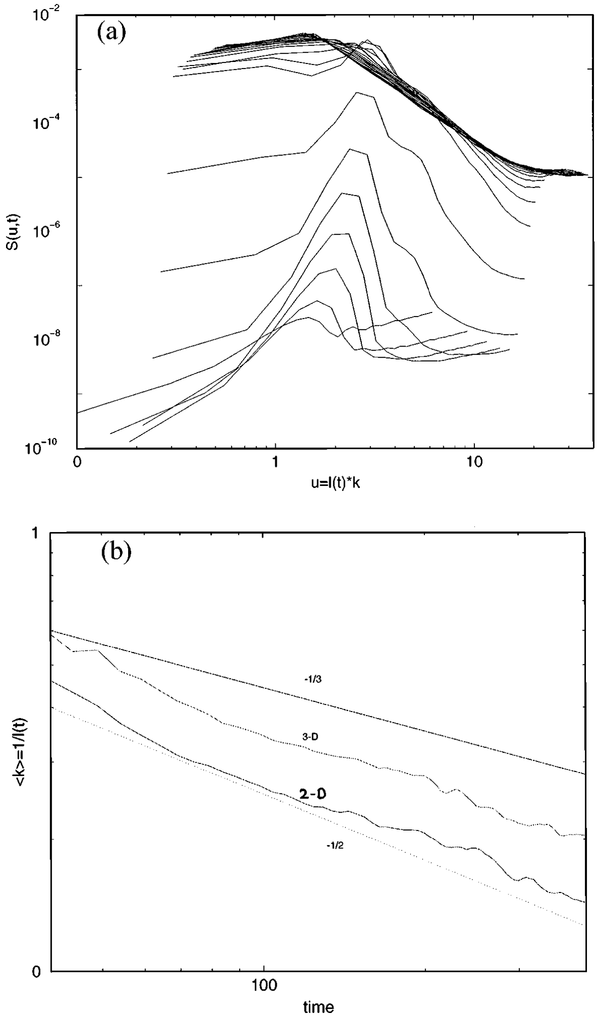

FIG. 2. (a) Log-log plot of $t^{-1}S(k,t)$ vs $t^{1/2}k$ at different equal times intervals, in 2D. The curves at the bottom represent the exponential growth in time of the focusing instability given by the linear equation $\partial_t S(k,t) = \sigma_k S(k,t)$. The nonlinearities saturate this exponential growth, and we can see that these functions reach a universal function, which for large u follow the Porod law in 2D, $S(u) \sim u^{-(D+1)}$, D being the space dimension. (b) For large t, the mean value $\langle k \rangle$, in 2D and 3D has been computed and one can note that the inverse of the characteristic length of our problem follows the scaling law $\langle k \rangle \sim t^{-1/D}$. This means that the number or bubbles in the system is inversely proportional to the time. All these simulations have been done with $\rho_c = 1.1$ and $\rho_0 = 1$.

Because of the slow coalescence or condensation of the small droplets, the final state is a unique solitary droplet. The long term evolution, with Dirichlet boundary conditions on ψ, makes the droplets disappear on the boundaries leading to a single droplet at the center of the box, presumably the structure of the ground state of the system. The excess energy transforms into vibrations of the droplet and small scale oscillations. We note that the central pulse has an internal excited mode of oscillation (the second angular harmonic), which persists as far as we could follow in numerical simulations. The

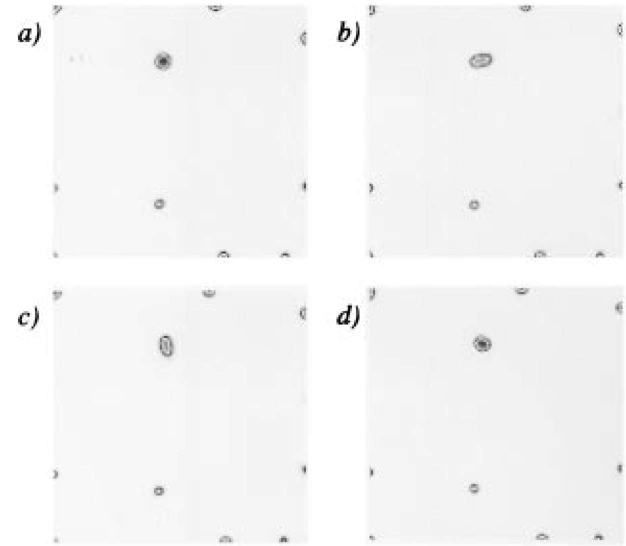

FIG. 3. A temporal sequence of a state dominated by oscillatory droplets as we see from (a) through (d).

frequency is given by the classical formula of Rayleigh for capillary oscillations [10] $\omega^2 = 6\alpha/\rho r_0^3$, α being the surface energy (per unit of mass) which we will discuss later and r_0 the radius of the droplet.

The first step to understand this two dimensional pulse is through the one dimensional case. We seek a solution of (2) of the form $R(x)e^{i\mu t}$, with $R(\pm x) \to 0$, for $x \to \infty$:

$$-\tfrac{1}{2} R_{xx} - 2\rho_c R^3 + R^5 + \mu R = 0 .$$

We obtain the known soliton solution of [11]:

$$R^2(x) = \frac{3\rho_c}{2} \frac{1 - a^2}{2a\cosh^2(\sqrt{2\mu}x) + 1 - a}, \tag{4}$$

where $a = \sqrt{1 - 4\mu/3\rho_c^2}$. The dimensionless parameter a characterizes completely the solitons.

By imposing that the total number of particles is equal to $N = \int_{-\infty}^{\infty} dx R^2(x)$, we get $\mu = (3\rho_c^2/4)\tanh^2 \sqrt{2/3}N$; thus, N is directly related to a by $a = 1/\cosh(\sqrt{2/3}N)$.

In the thermodynamic limit ($N \to \infty$) a goes to 0, i.e., $\mu \to 3\rho_c^2/4$, and the soliton tends to a front from $\rho = 0$ (at $x \to -\infty$) to $\rho = \frac{3}{2}\rho_c$ for a intermediate band (arbitrary large depending linearly on N) near $x = 0$, and then again $\rho = 0$ for $x \to \infty$. This value $\rho = \frac{3}{2}\rho_c$ is such that the equilibrium pressure is established, i.e., $p(\rho = 0) = p(\rho = \frac{3}{2}\rho_c) = 0$ [7], as we have explained for the coarsening process.

Let us come back to the surface energy between the liquid and the vapor in 2D. We can estimate this when the number of particles is large, i.e., $\mu \approx 3\rho_c^2/4$. We consider a one dimensional pulse between $\rho(x = -\infty, y, z) = 0$ and $\rho(x = 0, y, z) = \frac{3}{2}\rho_c$; thus, the surface energy is given by integration along x of the energy (3) (in fact at equilibrium we need the free energy

$H + \mu N$)

$$\alpha = \int_{-\infty}^{0} dx(\tfrac{1}{2} R_x^2 - \rho_c R^4 + \tfrac{1}{3} R^6 + \mu R^2) \equiv \int_{-\infty}^{0} dx R_x^2 = \frac{9\rho_c^2}{16\sqrt{6}}.$$

The soliton solution (4) is stable towards fluctuations in the x direction, as we shall now prove. We introduce a perturbation of the soliton solution (4): $\psi(x,t) = [R(x) + \delta\psi(x)e^{\sigma t}]e^{i\mu t}$ into Eq. (2). For small $\delta\psi$ we get the eigenvalue problem

$$\sigma\begin{pmatrix} \delta\psi_1 \\ \delta\psi_2 \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{L}_1 \\ -\mathcal{L}_2 & 0 \end{pmatrix}\begin{pmatrix} \delta\psi_1 \\ \delta\psi_2 \end{pmatrix}, \tag{5}$$

with $\mathcal{L}_1 = -\frac{1}{2}\partial_{xx} - 2\rho_c R^2(x) + R^4(x) + \mu$ and $\mathcal{L}_2 = -\frac{1}{2}\partial_{xx} - 2\rho_c R^2(x) + R^4(x) + \mu - 4[\rho_c R^2(x) - R^4(x)]$, two Hermitian operators.

As a consequence of the symmetries of the solution (4) of Eq. (2) the null space has at least dimension four [the three mentioned above plus a continuous symmetry of the solution (4) by the arbitrary choice of the initial total number of particles, which lead to an extra Goldstone mode].

The eigenvalues follow directly from the spectra of $i\sqrt{\mathcal{L}_1\mathcal{L}_2}$. We compute numerically the spectra getting four neutral modes with an eigenvalue equal to zero, and two continuous imaginary branches with a well defined frequency gap equal to μ. There is no eigenvalue with a real part for any set of parameter; thus, the soliton solution (4) is stable. However, transverse perturbations depending on the y and z coordinates are unstable. If we make $\delta\psi(x) \to \delta\psi(x)e^{iqy}$, the only change in the eigenvalue problem (5) is μ going to $\mu + q^2/2$. Thus, for the continuum part of the spectrum there is always a positive gap; however, the four neutral modes split in such a way that two of them develop a long wavelength instability in q. The growth rate increases as the wave number of the perturbation increases until a maximum, then the rate decreases to zero for a given wave number. Consequently, a transverse one dimensional soliton breaks down in 2D into droplets with a more or less well defined size.

Actually, the analytical stability of two dimensional droplets is more difficult because we do not know the shape of the soliton solution (probably, we may compute this solution only numerically). However, numerically, we can say that droplets are stable only as long as our numerical simulation ran (few thousand time units). Furthermore, the two dimensional pulses are unstable against perturbations in the third dimension, as is usual in the Rayleigh instability of a column of liquid in classical fluid dynamics [10], leading to stable 3D droplets.

Finally, it may be suggested that droplets in two dimensions are, furthermore, unstable against a small perturbation far from the main pulse, because of the focusing instability: The small perturbation tends to increase since the fifth power term is negligible; thus, one may imagine a final state made of many different droplets with a principal one. However, because of the coarsening process, these perturbations are evaporated, increasing the amount of matter in the main one. Another—more interesting—situation will be an array or crystal of droplets, and this situation is unstable for the same reason.

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