Vortex Lattice Formation in Bose-Einstein Condensates

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We show that the formation of a vortex lattice in a weakly interacting Bose condensed gas can be modeled with the nonlinear Schrödinger equation for both $T = 0$ and finite temperatures without the need for an explicit damping term. Applying a weak rotating anisotropic harmonic potential, we find numerically that the turbulent dynamics of the field produces an effective dissipation of the vortex motion and leads to the formation of a lattice. For $T = 0$, this turbulent dynamics is triggered by a rotational dynamic instability of the condensate. For finite temperatures, noise is present at the start of the simulation and allows the formation of a vortex lattice at a lower rotation frequency, the Landau frequency. These two regimes have different vortex dynamics. We show that the multimode interpretation of the classical field is essential.

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Vortex lattices exist in many domains of physics, from neutron stars to superconductors or liquid helium. In none of these systems has the formation of the lattice been understood at the level of a microscopic theory. Several groups have recently observed the formation of a vortex lattice in weakly interacting Bose gases [1–4] and are able to monitor this formation in real time. This gives us the chance to understand the problem of lattice formation in a relatively simple system. Indeed there have been theoretical attempts to understand the formation process [5–8] with simulations of the Gross-Pitaevskii equation for the condensate wave function. All of them stress the need for explicitly including a damping term representing the noncondensed modes to which the vortices have to give away energy to relax to a lattice configuration. In this Letter, we consider this problem in the framework of the classical theory of a complex field [9] whose exact equation of motion is the nonlinear Schrödinger equation (NLSE). First, we show that lattice formation is predicted within this framework without the addition of damping terms. Second, we provide two distinct scenarios of vortex lattice formation (dynamics, temperature dependence of the formation time, and critical rotation frequency) that can be directly compared with the experiments. We study the formation of the lattice in 3D from an initially nonrotating Bose condensed gas both at $T = 0$ and at finite temperature. Contrary to the common belief, we find that the dynamic instability, which was predicted in [10] to occur above a certain threshold value of the trap rotation frequency, leads to the formation of a vortex lattice. The formation time is in this case only weakly dependent of the temperature and the observed scenario and time scales are comparable to those seen in present experiments. For a lower trap rotation frequency corresponding to the Landau frequency, but only at finite temperature, we identify a new scenario not yet observed experimentally in which the vortices enter a few at a time and gradually spiral towards the center.

We start our simulations with the nonrotating classical field in thermal equilibrium. For $T = 0$, the system initially is a pure condensate and the field is proportional to the condensate wave function ϕ given by the Gross-Pitaevskii equation in the absence of rotation, $\psi = \sqrt{N_0}\phi$, where N_0 is the condensate atom number. For finite temperatures, we sample the initial thermal equilibrium in the Bogoliubov approximation at a given temperature T for a fixed number N_0 of condensate particles. In this approximation, the classical field is given by $\psi(\mathbf{r}, 0) = \sqrt{N_0}\phi(\mathbf{r}) + \psi_\perp(\mathbf{r})$. The random field $\psi_\perp(\mathbf{r})$ orthogonal to ϕ [11] representing the thermal noise is given by

$$\psi_\perp(\mathbf{r}) = \sum_n b_n u_n(\mathbf{r}) + b_n^* v_n^*(\mathbf{r}), \tag{1}$$

where u_n and v_n are the Bogoliubov mode functions associated with ϕ and b_n are independent random c numbers taken from a Gaussian distribution that obeys the classical equipartition formula, $\langle b_n^* b_n \rangle = k_B T/\epsilon_n$, ϵ_n being the Bogoliubov energy of mode n. In practice, to sample this distribution we use the Brownian motion method described in [11]. In our work, the field ψ is to be interpreted not as the condensate wave function but as the whole matter field. We present here results from single realizations of the field ψ which experimentally correspond to single runs. We have checked that different realizations lead to similar results.

In our simulations, we consider a Bose condensed gas initially trapped in a cigar-shaped harmonic potential with oscillation frequencies whose ratio is 1:1:0.25, with 10^5 atoms of mass m and a coupling constant $g = 0.0343$ in units of $\hbar\omega a_0^3$, where ω is the radial frequency and $a_0 = \sqrt{\hbar/m\omega}$ is the oscillator length. The corresponding chemical potential is $\mu = 8\hbar\omega$. We start each simulation with the gas in thermal equilibrium. We abruptly turn on the trap anisotropy which leads to a change in the radial frequencies: $\omega_{x,y}^2 = \omega^2(1 \mp \epsilon)$, where $\epsilon = 0.025$. Then

the rotation frequency $\Omega(t)$ of this anisotropy is slowly increased from zero to a final value Ω_f over $500\omega^{-1}$, to follow Procedure I in [10]. After that, we let the gas evolve in the presence of the rotating anisotropy until the angular momentum of the gas reached a steady state.

The calculation is performed in the rotating frame so that the NLSE takes the form

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r}) + g|\psi|^2 - \Omega(t)L_z\right]\psi, \quad (2)$$

where L_z is the angular momentum operator along z, and U is the anisotropic harmonic potential. The field ψ is subject to periodic boundary conditions in the rotating frame [12]. Our grid size is $32 \times 32 \times 128$ corresponding to an energy cutoff of $32\hbar\omega$ per spatial direction, although we have also run simulations on a $64 \times 64 \times 256$ grid (see below).

Zero initial temperature.—This set of simulations can be divided into two groups: those for which the final rotation frequency is $\Omega_f/\omega \leq 0.7$ and those with $\Omega_f/\omega \geq 0.75$. Between these two values lies the threshold for the dynamic instability of the condensate which changes the subsequent dynamics dramatically [10,13]. In the first group, as the rotation frequency gradually increases with time, the condensate adiabatically follows a steady state, apart from excitations of the surface modes leading to a very small oscillation of the angular momentum [see curve for $\Omega_f = 0.7\omega$ in Fig. 2(a) (below)]. With increasing Ω_f, the condensate's final state becomes more and more elliptically deformed, surrounded by a ring of vortices which, however, never enter it. The second group shows a completely different behavior when $\Omega(t)/\omega \simeq 0.75$ (see left column of Fig. 1): The instability sets in; the condensate becomes slightly S-shaped at $t \simeq 450\omega^{-1}$ before being highly deformed and undergoing very turbulent motion [5]. This is accompanied by a large increase in angular momentum of the gas from almost zero when $\Omega(t) < 0.75\omega$ to between $5\hbar$–$7\hbar$ per particle [see Fig. 2(a)]. At this point ($t \simeq 670\omega^{-1}$) several vortices enter the high density region and, in less than $200\omega^{-1}$, settle down to form a well-defined lattice. After this, a period of relaxation of around $800\omega^{-1}$ begins with the initially rotating lattice finally stopping in the rotating frame. There remains a small random motion of the vortices around their equilibrium positions in the lattice together with density fluctuations in and around the condensate.

At the end of the simulation, damping of the vortex motion has occurred and the initial energy of the vortex motion has been transferred in an effectively irreversible way to other degrees of freedom of the field. A similar phenomenon has been observed for the relative motion of two condensates [15]. *If we assume that the field has reached a thermal distribution*, we can calculate the temperature of the system by taking the final state of the simulation and evolving it with the conjugate gradient method in a trap rotating at Ω_f. This reduces its energy

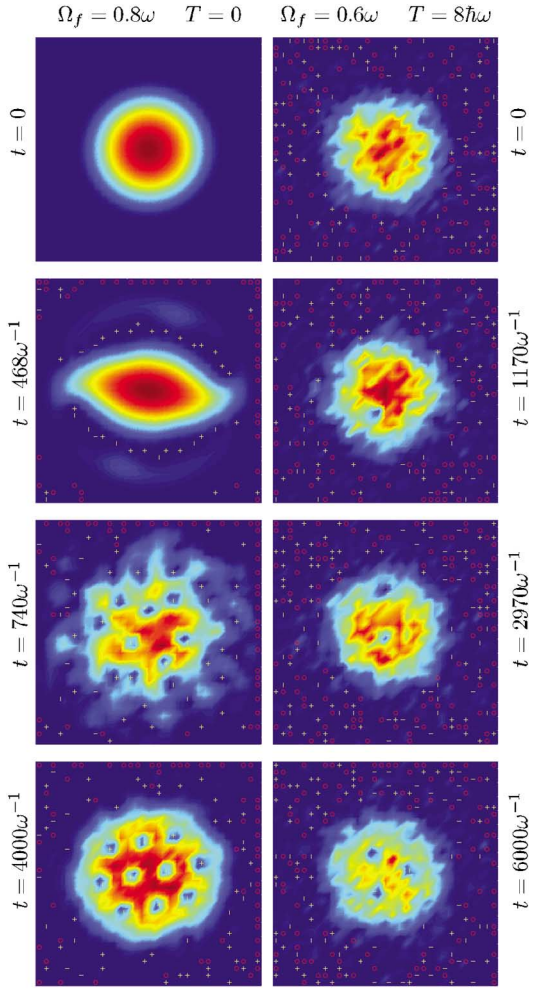

FIG. 1 (color online). Cut along the radial plane ($z = 0$) of the system spatial density at different times. Crosses (circles) indicate the position of vortices of positive (negative) charge [14]. Left column: $T = 0$, $\Omega_f = 0.8\omega$. Top to bottom: initial state; near instability; turbulent behavior; end of simulation. Right column: $k_BT = 8\hbar\omega$, $\Omega_f = 0.6\omega$. Top to bottom: initial state; entry of first vortex; entry of second vortex; end of simulation with a three-vortex lattice.

and takes it to the local minimum associated with the vortex lattice. We then calculate the energy difference ΔE between the final state of the simulation and the one at the minimum. Assuming that Bogoliubov theory is valid, ΔE must correspond to the energy of a classical thermal distribution of weakly coupled harmonic oscillators of amplitude b_n which obeys the equipartition formula $\langle b_n^* b_n\rangle\epsilon_n = k_BT$, with n being the Bogoliubov mode number. So, if $\mathcal{N}$ is the number of modes in the system (and keeping in mind that we have to subtract the one corresponding to the condensate), then we have

$$\Delta E = \sum_n \langle b_n^* b_n\rangle\epsilon_n = (\mathcal{N} - 1)k_BT. \quad (3)$$

The final temperature is $0.616\hbar\omega$ for $\Omega_f = 0.75\omega$ and $0.754\hbar\omega$ for $\Omega_f = 0.8\omega$, in other words it is extremely small, less than a tenth of the chemical potential.

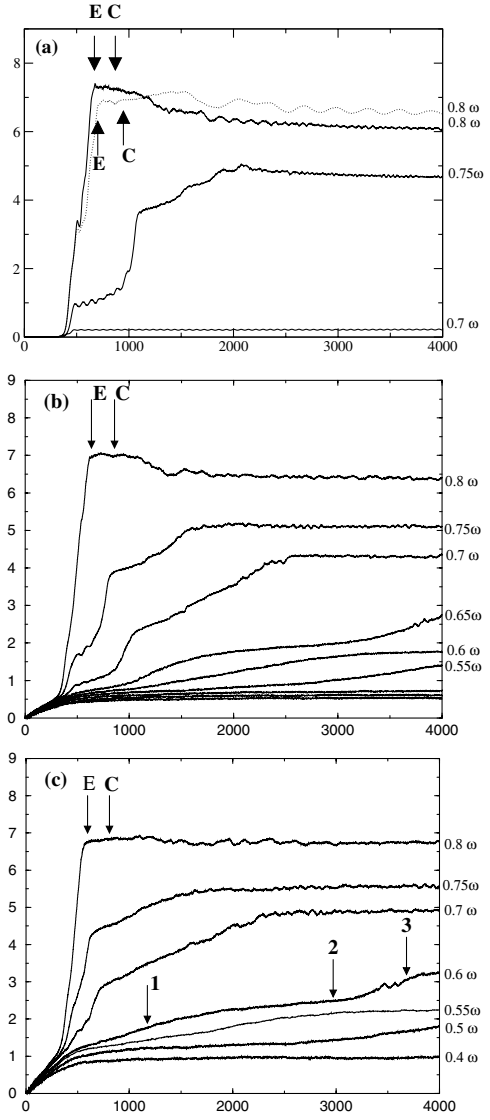

FIG. 2. Total angular momentum of the system in units of $\hbar$ per atom as a function of ωt. The arrows marked E and C indicate the entry of the vortices into the condensate and the crystallization of the lattice for $\Omega_f = 0.8\omega$. (a) $T = 0$, solid lines from bottom to top: $\Omega_f/\omega = 0.7(0), 0.75(7), 0.8(10)$; dashed line: $\Omega_f/\omega = 0.8(10)$ with a grid size of $64 \times 64 \times 256$. All other curves were done on a $32 \times 32 \times 128$ grid. In parenthesis is the number of vortices in the lattice at the end of the simulation. (b) $k_B T = 4\hbar\omega$, $\Omega_f/\omega = 0.4(0), 0.45(0), 0.5(0), 0.55(1), 0.6(1), 0.65(2), 0.7(6), 0.75(7), 0.8(10)$. (c) $k_B T = 8\hbar\omega$, $\Omega_f/\omega = 0.4(0), 0.5(1), 0.55(1), 0.6(3), 0.7(7), 0.75(7), 0.8(10)$. The arrows correspond to the approximate entry time of the vortices for $\Omega_f = 0.6\omega$ as shown in Fig. 1. Note that the total angular momentum shows no signature of the entries.

We have also carried out a simulation on a larger grid ($64 \times 64 \times 256$) to check the dependence on size. We chose $\Omega_f = 0.8\omega$ and compared it with the one on the $32 \times 32 \times 128$ grid. The vortex nucleation and crystallization phases are very similar and occur at roughly the same times. At longer times, two differences arise: First, there are large underdamped oscillations of the angular momentum [see Fig. 2(a)]. An analysis of the simulation suggests that these oscillations are those of the scissors mode. Second, the final temperature ($0.094\hbar\omega$) differs by the ratio of the number of modes as expected: At time $t = 500\omega^{-1}$ when $\Omega(t) = \Omega_f$, ψ had not yet reached the boundary in the smaller grid case and so the evolution of ψ on both grids was identical up to this time with the same total energy which was conserved at later times resulting in the same value of ΔE. This exemplifies the fact that, in classical field theories, the relationship between energy and temperature depends on the energy cutoff.

Since the thermal occupation of the modes is directly proportional to the temperature, we expect that all relaxation processes which involve scattering from or into those modes (such as Landau-Beliaev damping) will be reduced. We are thus led to the conclusion that, for our simulations starting at $T = 0$, relaxation rates in the period after the formation of the lattice could depend on the size of the grid. However, with the present numerical results, we were not able to demonstrate this.

Finite initial temperature.—We performed simulations starting with $k_B T = 4\hbar\omega$ and $k_B T = 8\hbar\omega$. Now not only the condensate but also other modes are occupied in the initial state, with a thermal distribution. For a final rotation frequency below that of the dynamic instability, the situation is quite different from that of the zero temperature case: The condensate is never deformed and the vortices do enter the condensate if $\Omega_f \geq 0.55\omega$ for $k_B T = 4\hbar\omega$ and if $\Omega_f \geq 0.5\omega$ for $k_B T = 8\hbar\omega$. In contrast to the $T = 0$ case at a frequency below that of the dynamic instability, all the noncondensed modes are now thermally occupied allowing the condensate to exchange particles, energy, and angular momentum with the noncondensed cloud. Therefore, as soon as Ω_f is greater than the Landau frequency (at which the vortex-free condensate is no longer a minimum of the energy [6]), the condensate moves gradually toward an energy minimum with one or more vortices. We have found numerically by imaginary time evolution that the Landau frequency is 0.51ω. During the real time evolution corresponding to $\Omega_f = 0.6\omega$ (right column of Fig. 1), we find that the vortices enter only one at a time. That is, as the angular momentum of the cloud increases, one vortex out of the group of vortices that surrounds the condensate will enter it and spiral slowly clockwise towards the center on a time scale of hundreds of ω^{-1}. After that vortex has reached the center, a second one enters slowly, repeating the trajectory of the first until it starts to interact with it, and the two orbit around each other for a while after which a third will enter. At the end of the simulation, coinciding with the achievement of the plateau in angular momentum, the lattice becomes stationary in the rotating frame and no further vortex enters the condensate. For $\Omega_f = 0.7\omega$, we find that the condensate deforms itself elliptically after which three vortices enter at the same time and form a rotating lattice. After that, and spaced by

several hundred ω^{-1}, a fourth and then a fifth vortex enter. Finally, two further vortices enter simultaneously to form the final seven vortex lattice. At each intermediate stage there is always a well-defined lattice present although it is not stationary in the rotating frame. We should contrast this with the scenario of [6,7], where a large number of vortices enter all at once into the condensate in a ring configuration and then some of them form a lattice while others are shed and leave the condensate.

For Ω_f above the dynamic instability frequency, the situation is quite similar to the corresponding one at $T = 0$. Once the instability has set in the lattice is formed for both temperatures in about $200\omega^{-1}$ as in the $T = 0$ case [see Figs. 2(b) and 2(c)]. This weak temperature dependence was also found experimentally [16]. We find a time for the lattice to stop rotating on the order of $100\omega^{-1}$, much shorter than at $T = 0$.

It is important to emphasize the multimode interpretation of the field. Transposing Penrose and Onsager's definition to the classical field theory, the condensate wave function is defined as the eigenvector corresponding to the largest eigenvalue of the one-body density matrix $\langle \psi^*(\mathbf{r}')\psi(\mathbf{r})\rangle$ where the average is over an ensemble of initial states. If the system becomes turbulent because it encounters an instability, the trajectories of the neighboring realizations will diverge exponentially. However, after averaging, we believe that the condensate wave function will not be a turbulent function. For $T = 0$, there is only one initial state and so we replace ensemble averaging by one over time in the steady state regime [17]. In our simulations with $\Omega_f = 0.8\omega$, the system must therefore be understood as becoming intrinsically multimode even though we started at $T = 0$ with a pure condensate. This shows that any theoretical model which singles out the condensate mode for separate treatment with a Gross-Pitaevskii–type equation could run into trouble in turbulent situations since the separation between condensed and noncondensed modes would be hard to keep.

Conclusions.—We have identified two very different scenarios for the crystallization of the vortex lattice in the classical field model. In the first one, the vortex and the subsequent lattice formation are triggered by a dynamic instability which sets in for a threshold value of the rotation frequency of the trap. Many vortices enter the condensate at the same time and settle into a lattice in about $200\omega^{-1}$. In this scenario, the lattice formation time is essentially the same for both $T = 0$ and finite temperatures in agreement with experimental observation [16]. In the second scenario, observed only at finite temperatures, vortices appear for a lower value of the rotation frequency corresponding to the Landau frequency, and so no dynamic instability occurs. The vortices enter one by one into the condensate and settle into a lattice before the entry of the following one. Thus far, there has been no experimental check of this second scenario.

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Note added.—We have been informed that crystallization of the vortex lattice has also been observed in a simulation without a damping term by the group of Bigelow [18].

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