Vortex crystallisation in classical field theory

Carlos Lobo, Alice Sinatra and Yvan Castin
Laboratoire Kastler Brossel, Ecole Normale Supérieure, 24 Rue Lhomond, 75231 Paris Cedex 05, France

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 an already known 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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Several groups have recently observed the formation of a vortex lattice in weakly interacting Bose gases \[1, 2, 3, 4\]. Theoretically there have been attempts to understand the formation process \[4, 5, 6, 7\] with simulations of the Gross-Pitaevskii equation for the condensate wavefunction. These papers either do not consider the effect of the noncondensed modes \[5, 8\] or they approximate it with an added damping term. All of them stress the need for explicitly including this term since the vortex lattice would be formed without the need for any dissipative term. The issue of relaxation to thermal equilibrium for purely Hamiltonian dynamics is analogous to the classical equipartition formula, \( \langle b_n^* b_n \rangle = k_B T/\epsilon_n \), \( \epsilon_n \) being the Bogoliubov energy of mode \( n \). In practice, to sample this distribution we use the Brownian motion method described in \[14\]. We present here results from single realisations of the field \( \psi \) which experimentally correspond to single runs. We have checked that different realisations 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 \( \omega \) 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 from an initially nonrotating Bose condensed gas both at \( T = 0 \) and at finite temperatures using the NLSE. We find that, contrary to the prevalent view, the lattice is formed in both cases without any need for a damping term which suggests that thermalisation takes place in our system.

We start our simulations with the nonrotating classical field in thermal equilibrium. For \( T = 0 \) the initial state is simply a pure condensate, that is, with a field proportional to the condensate wavefunction \( \phi \) 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 \( \psi(r, 0) = \sqrt{N_0} \phi(r) + \psi_{\perp}(r) \). The random field \( \psi_{\perp}(r) \) orthogonal to \( \phi \) \[12\] representing the thermal noise is given by

\[
\psi_{\perp}(r) = \sum_n b_n u_n(r) + b_n^* v_n^*(r)
\]

where the \( u_n \) and \( v_n \) are the Bogoliubov mode functions associated with \( \phi \) and the \( b_n \) are independent random \( \epsilon_n \) numbers taken from a Gaussian distribution that obeys the classical equipartition formula, \( \langle b_n^* b_n \rangle = k_B T/\epsilon_n \). In practice, to sample this distribution we use the Brownian motion method described in \[14\]. In our work, the field \( \psi \) is to be interpreted not as the condensate wavefunction but as the whole matter field (unlike \[5, 6, 7, 8\]). We present here results from single realisations of the field \( \psi \) which experimentally correspond to single runs. We have checked that different realisations 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 \( \omega \) 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: \( \omega_{2,3}^2 = \omega^2(1 + \epsilon) \) where \( \epsilon = 0.025 \). Then the rotation frequency \( \Omega(t) \) of this anisotropy is slowly increased from zero to a final value \( \Omega_f \) over \( 500 \omega^{-1} \), to follow Procedure I in \[15\]. After that we let the gas evolve in the presence of the rotating anisotropy until, for most of our simulations, 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

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

\[2\]
\[ \Omega = 0.8\omega \quad T = 0 \quad \Omega = 0.6\omega \quad T = 8\hbar\omega \]

where \( L_z \) is the angular momentum operator along \( z \) and \( U \) is the anisotropic harmonic potential. The field \( \psi \) is subject to periodic boundary conditions in the rotating frame. Our gridsize 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). We have checked that it is necessary to have time independent boundary conditions in the rotating frame: periodic boundary conditions in the lab frame arrest the rotation of the non-condensed gas. We have also checked that a pure condensate cannot be set into rotation by the effect of the boundary conditions only, since the condensate density is extremely weak at the borders of the grid for our choice of gridsize. The harmonic trap anisotropy is then a crucial element for the formation of the lattice.

FIG. 1: Cut along the radial plane (\( z = 0 \)) of the system spatial density at different times. Crosses (circles) indicate position of vortices of positive (negative) charge \[17\]. Left column: \( T = 0, \Omega_f = 0.8\omega \). Top to bottom: initial state; near instability; turbulent behaviour; end of simulation. Right column: \( k_B T = 8\hbar\omega, \Omega_f = 0.6\omega \). Top to bottom: initial state; entry of first vortex; entry of second vortex; end of simulation with a 3-vortex lattice.

FIG. 2: Angular momentum in units of \( \hbar \) per atom. The arrows marked E and C indicate the entry of the vortices into the condensate and the crystallisation 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 gridsize 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 angular momentum shows no signature of the entries.

\[ E_C = 0.8 \]
at }T = 0\text{ by triggering the dynamic instability of }[15].

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\text{ and those with }\Omega_f/\omega \geq 0.75.\text{ Between these two values lies the threshold for the dynamic instability of the condensate which changes the subsequent dynamics dramatically [12]. 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 period variation of the angular momentum (see curve for }\Omega_f = 0.7\omega\text{ in Fig 2a).}

With increasing }\Omega_f\text{, 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 completely different behaviour when }\Omega(t)/\omega \simeq 0.75\text{ (see left column of Fig 1). The instability sets in, the condensate becomes slightly S-shaped at }t \simeq 450\omega^{-1}\text{ before being highly deformed and undergoing very turbulent motion [4]. This is accompanied by a large increase in angular momentum of the gas from almost zero when }\Omega(t) < 0.75\omega\text{ to between }5\hbar-7\hbar\text{ per particle (see Fig 3a). At this point }t \simeq 670\omega^{-1}\text{ several vortices enter the high density region and, in less than }200\omega^{-1}\text{, settle down to form a well-defined lattice. After this, a period of relaxation of around }800\omega^{-1}\text{ 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 [13]. 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 using it with the conjugate gradient method in a trap rotating at }\Omega_f.\text{ This reduces its energy and takes it to the local minimum associated with the vortex lattice. We then calculate the energy difference }\Delta E\text{ between the final state of the simulation and the one at the minimum. Assuming that Bogoliubov theory is valid, }\Delta E\text{ must correspond to the energy of a classical thermal distribution of weakly coupled harmonic oscillators of amplitude }b_n\text{ which obeys the equipartition formula }\langle b_n^*\rangle = k_BT.\text{ So, if }\mathcal{N}\text{ 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}

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

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

We have also carried out a simulation on a larger grid }\left(64 \times 64 \times 256\right)\text{ to check the dependence on size. We chose }\Omega_f = 0.8\omega\text{ and compared it with the one on the }32 \times 32 \times 128\text{ grid. The vortex nucleation and crystallisation 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 2b). An analysis of the simulation suggests that these oscillations are those of the scissors mode. Second, the final temperature }0.094\hbar\omega\text{ differs by the ratio of the number of modes as expected: at time }t = 500\omega^{-1}\text{ when }\Omega(t) = \Omega_f\text{, }\psi\text{ had not yet reached the boundary in the smaller grid case and so the evolution of }\psi\text{ 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 }\Delta E.\text{ 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-Beljaev damping) will be reduced. We are thus led to the conclusion that, for our simulations starting at }T = 0\text{, relaxation rates in the equilibration 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_BT = 4\hbar\omega\text{ and }k_BT = 8\hbar\omega.\text{ 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\text{ for }k_BT = 4\hbar\omega\text{ and if }\Omega_f \geq 0.5\omega\text{ for }k_BT = 8\hbar\omega.\text{ We have checked numerically that }0.51\omega\text{ is the Landau critical frequency above which the vortex-free condensate is no longer a local minimum of the energy. During the real time evolution of the right column of Fig 2, corresponding to }\Omega_f = 0.6\omega\text{, 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 }\omega^{-1}.\text{ 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 (see right column of Fig 2d).}
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 $\omega^{-1}$, 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 lattice while others are shed and leave the condensate.

For $\Omega_f$ 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 Fig. 2, c—this weak temperature dependence was also found experimentally by [13]). The main difference is that the relaxation time for the lattice to stop rotating is much shorter, on the order of a hundred $\omega^{-1}$, not eight hundred.

It is important to emphasize the multimode interpretation of the field. Transposing Penrose and Onsager’s definition to the classical field theory, the condensate wavefunction is defined as the eigenvector corresponding to the largest eigenvalue of the one-body density matrix $\langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \rangle$ 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 realisations will diverge exponentially. However, after averaging, we believe that the condensate wavefunction 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 [14]. 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.

Conclusions: We have identified two very different regimes for the crystallisation of the vortex lattice in the classical field theory. At $T = 0$ when the dynamic instability sets in (for high enough $\Omega_f$), the vortices enter the condensate abruptly and settle into a lattice even if there is no dissipative term in the equation of motion. This scenario is consistent with the one found experimentally at the ENS [20] with comparable timescales. At finite temperatures, where $\Omega_f > 0$, add an explicit damping term, we see that the thermal classical field can provide the damping of the vortex motion on its own which leads to very different behaviour from that observed by those authors in that the vortices can enter one by one into the condensate and settle into a lattice before the entry of the following one. So far there has been no experimental check of this scenario. Finally, as the $T = 0$ case shows, 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 non-condensed modes would be hard to keep.

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