Characterization of nonequilibrium states of trapped Bose–Einstein condensates

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Abstract
The generation of different nonequilibrium states in trapped Bose–Einstein condensates is studied by numerically solving the nonlinear Schrödinger equation. Inducing nonequilibrium states by shaking a trap creates the following states: weak nonequilibrium, the state of vortex germs, the state of vortex rings, the state of straight vortex lines, the state of deformed vortices, vortex turbulence, grain turbulence, and wave turbulence. A characterization of nonequilibrium states is advanced by introducing effective temperature, Fresnel number, and Mach number.

Keywords: trapped bosons, vortex germs, vortex rings, vortex lines, vortex turbulence, grain turbulence, wave turbulence

(Some figures may appear in colour only in the online journal)

1. Introduction

The most widely studied nonequilibrium state of quantum fluids is quantum turbulence [1–5]. Recently, quantum turbulence has received much attention in the study of cold atomic systems, as can be inferred from the review articles [4–7]. The creation of strongly nonequilibrium atomic states of Bose–Einstein condensates by shaking a trap, as suggested in [8, 9], has made it possible to experimentally realize the quantum turbulence of cold atomic gases in harmonic traps (see reviews [5–7]) and in a box-shaped trap [10].

But quantum turbulence is not the sole nonequilibrium state that can be generated by shaking a trap. Other nonequilibrium states, such as grain turbulence and wave turbulence, can be generated in experiments and analyzed numerically by solving the nonlinear Schrödinger (NLS) equation [11–14].

An important question is: how would it be possible to ascribe a quantitative characteristic to different nonequilibrium states that could be generated in trapped Bose-condensed systems? For classical liquids, laminar and turbulent flows are distinguished by the Reynolds number \( \text{Re} = \frac{vL}{\nu} \), where \( v \) is a characteristic flow velocity, \( L \) is a characteristic linear system size, and \( \nu \) is the kinematic viscosity [15]. The characterization of flows by the Reynolds numbers is also applicable to quantum liquids, such as superfluid helium [16]. However, for cold atomic gases at low temperatures, viscosity is zero, so that the Reynolds number becomes infinite [17]. The Strouhal number \( \text{St} = \frac{fL}{v} \) can be used [18, 19] to describe the motion of obstacles through atomic superfluid gas, where \( f \) is the vortex shedding frequency. Various patterns of vortex shedding can arise in quantum fluids behind moving obstacles [20, 21].

However, characterizing various nonequilibrium states that could arise in trapped atomic Bose-condensed systems, without any obstacles, is a problem that remains unsolved.

The aim of the present paper is twofold. First, we thoroughly analyze what qualitatively different nonequilibrium states can appear in trapped Bose–Einstein condensates when the trapping potential is perturbed by time-dependent
modulation. Second, we suggest a quantitative characterization of all such states by three quantities—effective temperature, Fresnel number, and Mach number.

The use of the Fresnel number is motivated by the analogy between nonequilibrium states of atomic systems and optical phenomena in lasers, where the terms optical turbulence or photon turbulence are well known. The Mach number has also been used to characterize turbulent flows in geophysics, as is discussed in the book by Smits and Dussauge [22]. Fresnel numbers for trapped cold atoms have also been discussed in the context of superradiant Rayleigh scattering [23]. These analogies suggest that the characteristics referred to be useful for describing nonequilibrium states of trapped atoms.

Our goal is to model the behavior of a Bose–Einstein condensate by numerically solving the three-dimensional time-dependent NLS equation describing the system of Bose-condensed atoms [24]. The system parameters are chosen to exactly coincide with the recent experiments [25, 26] with $^{87}$Rb. This allows us to compare our numerical results with the available experimental data. But such a comparison is not the aim of the present paper, since this has already been conducted in our previous publications [12–14]. A good agreement between numerical and experimental data has been observed. In the present paper, we concentrate on a more detailed numerical investigation of arising nonequilibrium states, finding additional types of the states, such as vortex germs, vortex rings, and strongly deformed vortices that have not been observed in earlier publications [12–14].

The most important point of the present paper is the suggested novel characterization of nonequilibrium states. We illustrate this characterization by nonequilibrium states generated in trapped Bose–Einstein condensates. But this characterization, being formulated in general terms, can be applied to any other nonequilibrium states.

In a brief letter [13], we studied experiments with nonequilibrium trapped atoms and an interpretation of the experimentally observed states. The discussed experiments exhibit only three such states: separate vortices, vortex turbulence, and grain turbulence, while in the present paper, we accomplish a detailed numerical investigation of all possible nonequilibrium states, distinguishing eight different states: weak nonequilibrium, vortex germs, vortex rings, vortex lines, deformed vortices, vortex turbulence, grain turbulence, and wave turbulence. Also, it transpired that the injected energy, considered in [13], was not the most convenient quantity, and as such, we suggest here new characteristics.

Defining such dimensionless quantities as a Fresnel and Mach number is useful in that they allow for comparison between systems with different geometries and length scales and also between different physical systems. In this light, defining a Fresnel number for a BEC allows one to draw parallels between optical and atomic nonequilibrium states, such as turbulence.

The transitions between the observed nonequilibrium states are not sharp phase transitions, but they are gradual crossovers. However, each state is qualitatively different from the others, and as such they can be well distinguished from each other and classified as separate states. The gradual crossover transitions are typical for finite systems and for nonequilibrium phenomena [27].

2. The generation of nonequilibrium states

We choose the same setup as has been used in recent experiments [25, 26] with $^{87}$Rb. At the initial moment of time, all atoms of $^{87}$Rb, with mass $m = 1.445 \times 10^{-22} \text{g}$ and a scattering length $a_s = 0.577 \times 10^{-6} \text{cm}$, are assumed to be Bose-condensed in a cylindrical harmonic trap with a radial frequency of $\omega_r = 2\pi \times 210 \text{Hz}$ and an axial frequency of $\omega_z = 2\pi \times 23 \text{Hz}$. The total number of atoms is $N = 1.5 \times 10^5$. The atomic cloud has a radius of $R_{\text{eff}} = 4 \times 10^{-4} \text{cm}$ and a length of $L_{\text{eff}} = 6 \times 10^{-3} \text{cm}$. The central density is $\rho = 2.821 \times 10^{14} \text{cm}^{-3}$. The healing length is $\xi = 1.106 \times 10^{-5} \text{cm}$.

As usual, for numerical calculations, it is convenient to write the time-dependent equation in a dimensionless form, with the energies measured in units of the characteristic oscillator frequency $\omega_0 = \left(\omega_r^2 \omega_z^2\right)^{1/3}$, time measured in units of $\omega_0^{-1}$, and lengths measured in units of the characteristic oscillator length $l_0 = \sqrt{\hbar/m\omega_0}$. Here $\omega_0 = 630 \text{ s}^{-1}$ and $l_0 = 1.08 \times 10^{-4} \text{cm}$.

Starting from the initial time, the trap is subject to the action of a perturbing alternating potential, such that the trapping potential, in dimensionless units, takes the form

$$V(\mathbf{r}, t) = \frac{1}{2} \left\{ \frac{1}{\alpha} \left[ x \cos \theta_1 + y \sin \theta_1 - z \sin \theta_2 - \delta_1 (1 - \cos \omega t) \right]^2 + \left[ y \cos \theta_1 - x \sin \theta_1 - \delta_2 (1 - \cos \omega t) \right]^2 + \left[ z \cos \theta_2 + x \sin \theta_2 - \delta_3 (1 - \cos \omega t) \right]^2 \right\} .$$

Here $\alpha \equiv \omega_0/\omega_r$ is the aspect ratio, $\delta_1 = A_1(1 - \cos \omega t)$, $A_1 = \pi/60$, $A_2 = \pi/120$, $\delta_1 = 1.861A$, $\delta_2 = 4.653A$, $\delta_3 = 2.792A$, the effective modulation amplitude $A = 0.2$, and the modulation frequency is $\omega = 2\pi \times 200 \text{Hz}$. These parameters could be varied, which, as we have checked, does not qualitatively change the overall picture. So, in numerical calculations, we keep them as defined above. The alternating trapping potential shakes the atomic cloud without imposing a moment of rotation.

The dynamics of the trapped Bose condensate is analyzed by numerically solving the NLS equation defined on a three-dimensional Cartesian grid. The grid contains $230^3$ points, and its mesh size is approximately half the healing length. As usual, for numerical calculations, it is convenient to write the time-dependent equation in a dimensionless form, with the energies measured in units of the characteristic oscillator frequency $\omega_0 = \left(\omega_r^2 \omega_z^2\right)^{1/3}$, time measured in units of $\omega_0^{-1}$, and lengths measured in units of the characteristic oscillator length $l_0 = \sqrt{\hbar/m\omega_0}$. Here $\omega_0 = 630 \text{ s}^{-1}$ and $l_0 = 1.08 \times 10^{-4} \text{cm}$.

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The dynamics of the trapped Bose condensate is analyzed by numerically solving the NLS equation defined on a three-dimensional Cartesian grid. The grid contains $230^3$ points, and its mesh size is approximately half the healing length. This set of parameters allows us to avoid the unphysical reflection from the grid boundaries and properly simulate all nonequilibrium states. Energy dissipation is taken into account by introducing a phenomenological imaginary term into the left-hand side of the NLS equation. For more detailed information regarding the numerical procedure, we refer readers to [28].

In the process of perturbation, different spatial structures appear, such as vortex germs, vortex rings, vortex lines, and grains. The lifetime of these structures is defined in the following way. After they are created, the external pumping is switched off and the behavior of the structures in the stationary trap is monitored.
The sequence of the observed nonequilibrium states is as follows.

(i) Weak nonequilibrium. At the first stage of the process, lasting around 5 ms, the energy injected into the system is not yet sufficient to generate topological modes, but produces only density fluctuations above the equilibrium state of the atomic cloud.

(ii) Vortex germs. After 5 ms of perturbation, at the low-density edges of the cloud, pairs of vortex germs appear that resemble broken pieces of vortex rings. These objects do possess vorticity \( \pm 1 \), which is found by reconstructing vortex lines in the coordinate space employing the method described in [4, 29]. According to this method, the points are defined representing the location of phase defects in the three-dimensional coordinate space and thus defining the position of the vortex core. It is assumed that the vortex line passes through the nearest points of the phase defects. If the external pumping is switched off after the germs are created, they survive for about 0.2 s, when they do not move, exhibiting only small oscillations. But if we continue pumping the energy into the trap, we proceed to the next stage. Typical vortex germs are shown in figure 1, where the related modulation time is marked.

(iii) Vortex rings. After around 10 ms, instead of vortex germs, well defined pairs of vortex rings appear, with vorticity \( \pm 1 \). Typical examples of vortex rings are illustrated in figure 2, where the modulation time is also marked. The rings do not move, exhibiting only small oscillations. The ring lifetime, after switching off pumping, is about 0.1 s.

(iv) Vortex lines. Continuing pumping energy into the system leads, after about 15 ms, to the formation of pairs of straight vortex lines, with vorticity \( \pm 1 \), directed along the \( z \)-axis, as is demonstrated in figure 3. The lines randomly move, probably due to the Magnus force. The vortex lifetime, after switching off pumping, is about 0.2 s.

(v) Deformed vortices. The longer perturbation, after around 17 ms, starts strongly deforming vortex lines, making them deformed and chaotically directed. The lifetime of the deformed vortices is close to that of the straight vortex lines.

(vi) Vortex turbulence. After about 25 ms, the number of deformed vortices sharply increases and they form a randomly oriented vortex tangle, typical of Vinen turbulence [2–4, 30]. The total regime of vortex turbulence can be subdivided into the stages of developing turbulence, developed turbulence, and decaying turbulence. The stage of developed vortex turbulence is demonstrated in figure 4. The regime of vortex turbulence can be classified as such, since it exhibits several features typical of quantum turbulence. First, a random tangle of vortices appears, corresponding to the definition of quantum turbulence by Feynman [31]. Second, being released from the trap, the atomic cloud expands isotropically, which is typical of Vinen turbulence [32]. Third, the column-integrated radial momentum distribution obeys a power law \( n_r(k) \propto k^{-\gamma} \) in the range [4] \( k_{\text{min}} < k < k_{\text{max}} \), with \( k_{\text{min}} \approx \pi / \xi \) and \( k_{\text{max}} \approx 2\pi / \xi \); which is a key quantitative expectation for an isotropic turbulent cascade [33], and which has been observed for the turbulence of trapped atomic clouds [10, 34]. We have found that in this range, \( 0.284 \times 10^6 \text{ cm}^{-1} < k < 0.568 \times 10^6 \text{ cm}^{-1} \), the slope of \( n_r(k) \) is \( \gamma \approx 1.7 \), which is close to \( \gamma \approx 2 \) found in the experiment [34] accomplished for the same system with the same parameters.

(vii) Grain turbulence. The regime of decaying vortex turbulence, after approximately 40 ms, is followed by a state where there are practically no vortices, but the whole trap is filled with dense Bose-condensed droplets or grains randomly distributed in space, surrounded by a rarified gas. The droplets are almost spherical, with a radii of \( (0.5–2.5) \times 10^{-5} \) cm. The typical droplet radius of \( 1.5 \times 10^{-5} \) cm is close to the coherence length, as it should be. The density inside a droplet is 20–100 times higher than in the surrounding gas. The lifetime of a grain, after switching off pumping, is about 0.01 s. During this time, droplets chaotically move in space, then some of them disappear, while new ones appear. The droplet lifetime is much longer than the local equilibration time \( t_{\text{eq}} = m / \hbar \rho u_0 = 0.8 \times 10^{-3} \) s. Hence the droplets are metastable objects. Each droplet is coherent, having a constant phase, while in the surrounding gas the phase is random. Such a state can be treated as a heterophase mixture of Bose-condensed droplets immersed into the gas of uncondensed atoms [35, 36]. The density snapshot for a radial cross-section, comparing the state of grain turbulence with the equilibrium unperturbed condensate and with the following state of wave turbulence, is shown in figure 5. It is important to stress that the granulated state of matter, to be classified as such, must satisfy the following criteria: (1) the typical size of each droplet, representing a coherent formation, is of the order of the healing length; (2) the phase inside a droplet is constant, as it should be for a coherent object; (3) the phase in the space around a droplet is random so that the coherent droplets are separated from each other by incoherent surroundings; (4) the lifetime of a droplet is much longer than the local equilibration time, which defines the droplets as metastable objects; (5) to observe a droplet inside a rarified gas, the density inside a droplet should be much larger than that of its incoherent surroundings. If these criteria are not satisfied, the matter cannot be classified as granulated. In our case all these criteria hold true.

(viii) Wave turbulence. Increasing perturbation by the trap modulation destroys Bose-condensed droplets after about 150 ms and the system transfers into a state of wave turbulence [37, 38]. The state is a collection of small-amplitude waves, with the sizes \( (0.5–1.5) \times 10^{-4} \) cm and with a density only about three times larger than the density of their surroundings. There is no coherence either inside a wave or between them, since the phase is random. Strictly speaking, the transition from the regime of grain turbulence to wave turbulence is a gradual crossover, with more and more destroyed coherence. The latter is almost completely destroyed at about 150 ms, so that the phase is everywhere chaotic. A density snapshot of the state is demonstrated in figure 5.
3. Quantitative characterization of nonequilibrium states

In this way, by injecting energy into the trap, we create different nonequilibrium states with various topological defects, finally transforming an initial equilibrium Bose-condensed system into a state where the Bose–Einstein condensate is completely destroyed. This process, being opposite to equilibration, can be treated as an inverse Kibble–Zurek scenario [14]. The remaining problem is whether it is possible to quantitatively characterize the nonequilibrium states arising during this disequilibration process. Several characteristics can be suggested for such a characterization.

First of all, it is possible to check that the energy pumped into the system contributes almost completely to an increase in kinetic energy [14]. The latter can be connected to the effective temperature. Therefore, it is natural to define the effective temperature, in energy units by the increase of kinetic energy per atom from the initial value $E_{\text{kin}}(0)$ to its value $E_{\text{kin}}(t)$ at time $t$,

$$T_{\text{eff}}(t) \equiv \frac{2}{3} \left[ E_{\text{kin}}(t) - E_{\text{kin}}(0) \right].$$

Note that this expression is written in energy units. To obtain the units of Kelvin temperatures, one has to divide equation (2) by the Boltzmann constant $k_B$.

Another idea comes to mind if we remember that the phenomenon of turbulence is very general, arising in different media. Stochastic vortex tangles exist in many physical fields of similar systems of highly disordered sets of one-dimensional topological objects. For example, it is possible to mention global cosmic strings, the flux tubes in superconductors, dislocations in solids, linear topological defects in liquid crystals and polymer chains, turbulent effects in quark-gluon plasma and neutron stars (see the discussion in [4, 5]). The emergence of multiple random filamentation in a high-intensity, ultrashort laser beam, due to optical turbulence, has been observed [39–42]. The phenomenon of photon turbulence, or optical turbulence, also occurs in high-Fresnel-number lasers, where an increase in the laser Fresnel number leads to the appearance of turbulent photon filamentation [43–45].

Therefore, the Fresnel number can serve as a characteristic of the system state. For lasers with wavelength $\lambda$, radius $R$, and length $L$, the Fresnel number is $F = \pi R^2/\lambda L$. For atomic traps, the role of the radius is played by the oscillator length $R = l_r = \sqrt{\hbar/m\omega_r}$, while the axial length is given by $L = 2l_z = 2\sqrt{\hbar/m\omega_z}$. For the wavelength, it is natural to accept the length $\lambda_T = h\sqrt{2\pi/mT_{\text{eff}}}$. Thus, the effective Fresnel number can be written as

$$F = \frac{\pi R^2}{\lambda_T L} = \sqrt{\frac{\pi \alpha T_{\text{eff}}}{8\hbar\omega_r}},$$

where $\alpha$ is the aspect ratio.

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It is also possible to collect that turbulence is connected to such a characteristic as the Mach number $M = v/c$, in
which $v$ is the velocity of a moving object and $c$ is the sound velocity \cite{22}. For atomic systems, the velocity of an atom can be represented as $v = \sqrt{\frac{2E_{\text{kin}}}{m}}$ and the sound velocity can be written as $c = (\hbar/m)\sqrt{\frac{4\pi\rho}{\hbar}}$, where $\rho$ is the density at the trap center. Hence the effective Mach number takes the form

$$M = \sqrt{\frac{2E_{\text{kin}}}{mc^2}} = \frac{1}{\hbar} \sqrt{\frac{mE_{\text{kin}}}{2\pi\rho}}. \tag{4}$$

The first expression here is what is called the turbulence Mach number \cite{22}.

In general, the Mach number shows the relation between the object velocity and the speed of sound. Considering an obstacle, for example, a laser beam moving through the fluid, is a particular case. In our study, the Mach number characterizes the relation between the characteristic velocity of atoms and the speed of sound. The Mach number we introduce describes how a particle moves inside the system. In that sense, a particle is also an effective moving object, similar to an obstacle. So, the suggested definition is a straightforward generalization of the standard Mach number. Recall that cold atoms, we consider, are not thermal. Their speed has no connection with thermal motion, but reflects the speed due to quantum kinetic energy. In the case of cold atoms, kinetic energy is caused by quantum motion, while for classical systems kinetic energy
is really thermal. This is the principal difference between quantum and classical systems.

In figure 6, we illustrate the classification of all nonequilibrium states we have found by means of the effective temperature, Fresnel number, and Mach number. It is interesting that the regime of wave turbulence, where all coherence is destroyed, corresponds to the effective temperature $T_{\text{eff}} = 23.5 \hbar \omega_r$, which practically coincides with the temperature $T_c = 23.8 \hbar \omega_r$ of Bose–Einstein condensation of $^{87}$Rb in the considered setup. The critical temperature in Kelvin degrees is $2.4 \times 10^{-7}$ K. The developed wave turbulence implies that, although the system is yet quantum, there is no coherence, as it should be above the condensation temperature. The Fresnel and Mach numbers vary between small values close to zero in weak nonequilibrium, to values close to one in wave turbulence.

Note that for a strongly nonequilibrium system, the standard notion of temperature is not defined, but one can speak only about an effective temperature, as we do. The closeness of the effective temperature at the moment, when the coherence is destroyed by perturbations, to the Bose condensation temperature, implies that coherence can be destroyed either by heating an equilibrium system or by injecting kinetic energy into a nonequilibrium system, for which heating has no meaning.

4. Conclusion

In conclusion, we have accomplished a detailed numerical investigation of nonequilibrium states arising in the process of perturbing the Bose–Einstein condensate of trapped atoms by an alternating potential. Starting from an equilibrium
condensate, we generate the state of weak nonequilibrium, the states with vortex germs, vortex rings, vortex lines, and with deformed vortices, vortex turbulence, grain turbulence, and wave turbulence. The characterization of the nonequilibrium states is suggested by means of the effective temperature, Fresnel number, and Mach number. The latter are well defined quantities expressed through the known system parameters and kinetic energy that can be straightforwardly calculated numerically as well as measured experimentally. The overall physical picture remains the same if the perturbation parameters are varied. This is because the main characteristics of the states depend on whether the injected kinetic energy that can be shown [12–14] is proportional to the product $A\omega t$ of the modulation amplitude $A$, modulation frequency $\omega$, and modulation time $t$. So, the same amount of kinetic energy can be injected into the trap by increasing the modulation amplitude, but decreasing the modulation time or modulation frequency.

The suggested characteristics can be used for the traps of any geometry and for any type of cold atoms. The main definitions of the effective temperature, Fresnel number, and Mach number remain the same, although the expressions for the system sizes $R$ and $L$, as well as for the sound velocity $c$, can be different, depending on the trap geometry and system parameters. For example, in the case of a cylindrical box [10], the system sizes are given by the radius $R$ and length $L$ of the box.

It is important to emphasize that the characterization of nonequilibrium states proposed in the present paper is very general and can be employed for all systems for which such straightforward quantities as kinetic energy and the system sizes can be defined. These quantities, as is evident, can be defined for practically any experimental scheme. The suggested characteristics can be measured in experiments, provided kinetic energy can be measured. The latter can be found by measuring the momentum distribution $n(\mathbf{k})$, as in the experiments with trapped atoms [34, 46], after which the kinetic energy is straightforwardly obtained by integrating over momenta the expression $(k^2/2m)n(\mathbf{k})$.

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