Kinetics of Strongly Non-Equilibrium Bose-Einstein Condensation

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We consider the ordering kinetics in a strongly non-equilibrium state of a (weakly) interacting Bose gas, characterized, on one hand, by large occupation numbers, and, on the other hand, by the absence of long-range order. Up to higher-order corrections in inverse occupation numbers, the evolution is described by non-linear Schrödinger equation with a turbulent initial state. The ordering process is rather rich and involves a number of qualitatively different regimes that take place in different regions of energy space. Specially addressed is the case of evolution in an external potential.

I. INTRODUCTION

Kinetics of Bose-Einstein condensation (BEC) in a weakly interacting Bose gas is one of the most fundamental problems of non-equilibrium statistical mechanics. The exciting progress in the experiment with BEC in ultracold gases initiated by the pioneer works [1] opens up an opportunity of laboratory study of non-trivial regimes of BEC kinetics.

From the very beginning it should be realized that the statement of the problem of BEC kinetics involves a number of aspects that are of crucial importance to the very character of the evolution process. The nature of the process strongly depends on how the BEC is being achieved: Say, by slow cooling, or by self-evolution of an essentially non-equilibrium initial state. More generally, it is important to take into account whether the considerable deviation from equilibrium occurs only at some sufficiently large length scales and only in the fluctuation region (so that the kinetics is of universal character and does not reflect specifics of weakly interacting system), or the non-equilibrium situation arises far enough from the critical region and the resulting ordering kinetics is characteristic only to weakly interacting gas. Obviously, the picture of evolution can be “trivialized” if some portion of condensate is already present in the initial state. Finally, and especially importantly for the realistic case of a trapped gas, finite size of the system, or just only that of the condensate can partially or completely change the relaxation scenario, if this size turns out to be less than some correlation length relevant to the ordering process in the infinite system.

In this paper we concentrate on a statement of BEC kinetics problem that we believe to be the most characteristic of the case of weakly interacting gas. Namely, we consider the self-evolution of weakly interacting gas with a strongly non-equilibrium initial state. To maximally simplify the consideration without qualitatively changing the nature of the process, we assume that in the initial state all occupation numbers are either much larger than unity, or equal to zero, and that there are no correlations between different single-particle modes. The advantage of choosing such an initial condition is that from the very beginning one can employ classical-field description in terms of non-linear Schrödinger equation (NLSE), which in the theory of Bose gases is known as Gross-Pitaevskii equation [2], with a certain turbulent initial condition. It should be stressed that, in contrast to a wide-spread prejudice, the very description in terms of NLSE does not imply the presence of condensate, or any sort of dynamical phase transition (see, e.g., discussion in [3]). The question of the presence of condensate, or, more generally, the question of (long-range) order is the question of the (long-range) structure of corresponding classical field.

Hence, the dynamical model for our problem reads ($\hbar = 1$)

$$i \frac{\partial \psi}{\partial t} = -\frac{\Delta}{2m} \psi + V(\vec{r})\psi + U | \psi |^2 \psi,$$  

(1)

where $| \psi |^2$ is interpreted as particle density (not the condensate density!), $m$ is the particle mass, $V(\vec{r})$ is the external potential; $U = 4\pi a/m$ is the vertex of the effective pair interaction, $a$ is the scattering length. To introduce the initial condition to (1) one has to consider the expansion of $\psi(\vec{r}, t)$ in terms of eigen modes $\varphi_{\varepsilon}(\vec{r})$ $[(\Delta/2m + V)\varphi_{\varepsilon} = \varepsilon \varphi_{\varepsilon}]$ of linear part of NLSE: $\psi(\vec{r}, t) = \sum_{\varepsilon} a_{\varepsilon}(t)\varphi_{\varepsilon}(\vec{r})$. Then, at the initial moment $t = 0$, the phases of the complex amplitudes $a_{\varepsilon}$ can be considered as random, while $| a_{\varepsilon} |^2$ is identified with the occupation number $n_{\varepsilon}$ of the mode $\varepsilon$ (see, e.g., [3] for more details). To the best of our knowledge, the first formulation of BEC kinetics problem in terms of NLSE was given in [4].

A full-scale numeric simulation of NLSE with the turbulent initial condition could, in principle, cross almost all the $t$’s in the strongly non-equilibrium BEC kinetics problem. Such a simulation has not been done yet [4]. Nevertheless, we will see that from general considerations it is possible to propose the evolution scenario and to obtain all relevant estimates.
In very general terms, the direction in which the field \( \psi \) will evolve is clear from the following considerations. First, it is natural to expect that the system must relax to a certain equilibrium state. Secondly, this equilibrium state should correspond to zero temperature, since the classical field described by the equation \( f \) forms a heatbath at absolute zero with respect to itself. Hence, if there is a stable groundstate (that is if \( U > 0 \)) for a given particle density, then the system should approach it in this or that way, the excess energy being carried away (to higher and higher harmonics) by ever decreasing portion of high-frequency fraction of the field. At the final stage of evolution all the particles are condensed except for an infinitesimally small high-frequency portion.

Though the general tendency of evolution is clear, the particular relaxation scenario is not at all self-evident. A detailed analysis \( [4] \) leads to a rather sophisticated scenario that involves a number of qualitatively different stages. The evolution starts with an explosion-like wave in energy space, propagating from higher energies towards the lower ones, that leads to a formation of a specific power-law distribution of particles. Immediately after its formation, this distribution starts to relax. Simultaneously, in the low-energy region the so-called coherent regime sets in that leads to the formation of quasi-condensate correlation properties. Basically, the quasi-condensate state corresponds to what is known in the theory of superfluidity as the state of superfluid turbulence. It can be viewed as a condensate containing a tangle of vortex lines (plus a specific sharply non-equilibrium distribution of long-wave phonons). The formation of the quasicondensate occurs very rapidly (characteristic time is much smaller than the time of the wave formation). In contrast to it, the final stage of long-range ordering, associated with relaxing superfluid turbulence and long-wave phonons, takes a macroscopically large time.

In the present paper we render the homogeneous BEC scenario \( [6–8] \) (sections \( [4] \) and \( [1] \)) and project it onto the case of a trapped gas. We find out that in an external potential the evolution picture can be even more rich.

## II. KINETIC REGIME

During some initial period of evolution the correlations between different amplitudes \( a_\varepsilon \) are vanishingly small. Such a regime (known in the theory of non-linear classical-field dynamics as weak turbulence \( [9] \)) admits a description in terms of kinetic equation. This stage is thus referred to as kinetic stage.

Kinetic equation corresponding to the weak-turbulence regime of non-linear Schrödinger equation belongs to a generic class of scale-invariant models with four-wave particle- and energy-conserving interaction, that allows an analysis of evolution kinetics in general terms (see, e.g., \( [11] \)). For the BEC kinetics the analysis suggests that there are two alternative ways of the initial evolution: (i) shrinking of the particle distribution as a whole towards \( \varepsilon = 0 \) (during infinite time), or (ii) a specific wave in the energetic space leading to a singularization of distribution at the point \( \varepsilon = 0 \) at some finite time moment \( t = t_* \). The answer to the question of which scenario takes place for a given model depends only on the scaling properties of the collision integral and the density of states; and the case of NLSE corresponds to the scenario (ii).

The evolution at the beginning of the kinetic stage results in the formation of self-similar wave in the energy space propagating in an explosion-like fashion from the high-energy region (where the particles are initially distributed) towards lower energy scales. Corresponding self-similar solution of the kinetic equation has the form \( n_\varepsilon(t) = A\varepsilon^{-\alpha}(t)f(\varepsilon/\varepsilon_0(t)), \quad t \leq t_* \),

\[
n_\varepsilon(t) = A\varepsilon^{-\alpha}(t)f(\varepsilon/\varepsilon_0(t)), \quad t \leq t_* \tag{2}
\]

\[
\varepsilon_0(t) = B |t_* - t|^{1/2(\alpha - 1)} \tag{3}
\]

Here \( A \) and \( B \) are dimensionless constants depending on the initial condition and related to each other by the formula \( B = \text{const}(m^3/\hbar^2 A^2)^{1/2(\alpha - 1)} \). The dimensionless function \( f \) (numeric data for \( f \) see in \( [11] \)) is defined up to an obvious scaling freedom. The explosion character of the evolution guarantees that the wave reaches the point \( \varepsilon = 0 \) at some finite time moment \( t = t_* \) [\( t = 0 \) corresponds to the beginning of evolution], the value of \( t_* \) being on the order of the typical time of (stimulated) collisions in the gas at \( t = 0 \). Physically, this explosion-like evolution is supported by the stimulation of the collision rate at the head of the wave, \( \varepsilon \sim \varepsilon_0 \), by ever growing occupation numbers.

Generally speaking, the index \( \alpha \) in \( (2)-(3) \) cannot be established from the scaling properties of the collision term of the kinetic equation, being related thus to the particular form of the latter. It is possible, however, to specify lower and upper limits for \( \alpha \) following from the consistency of \( (2) \) and \( (3) \) with the requirement that these formulae describe an explosion-like singularization of distribution (rather than infinite-time shrinking). To this end we note that from the scale invariance it follows that \( f(x) \) behaves like some power of \( x \) at \( x \gg 1 \). At \( t = t_* \) the occupation numbers have to be finite at \( \varepsilon > 0 \), hence

\[
f(x) \rightarrow x^{-\alpha} \text{ at } x \rightarrow \infty. \tag{4}
\]
The requirement that the particle distribution does not shrink as a whole implies that the number-of-particles integral for the distribution (3) is divergent at $\varepsilon \to \infty$. This immediately yields $\alpha < 3/2$. The condition $\alpha > 1$ is necessary for $\varepsilon_0$ to approach zero at $t = t_\ast$. So we have $1 < \alpha < 3/2$. The most accurate up-to-date numeric analysis of $\alpha$ was performed in [10] with the result $\alpha \approx 1.24$.

At $t > t_\ast$, kinetic description is still valid for not so small energies, but to obtain an adequate sewing with the solution (3) one has to explicitly introduce the (quasi)condensate, employing the conservation of the total number of particles (see the discussion in [8]). The structure of the self-similar solution

$$n_\varepsilon(t) = A\varepsilon_0^{-\alpha}(t)\tilde{f}(\varepsilon/\varepsilon_0(t)), \quad \varepsilon > 0, \quad t \geq t_\ast$$

\[\tilde{f}(x) \to f(x) \quad \text{at} \quad x \to \infty\] corresponds to a back wave in the energy space, destroying the singular distribution created by the wave (3). The particles being released during this destruction go directly to quasicondensate. For the quasicondensate density $n_0$ we thus have

$$n_0(t) = \frac{A}{4\pi^2}(2m)^{3/2}\varepsilon_0^{-3/2-\alpha}(t)\int_0^\infty dx\sqrt{x|x^{-\alpha} - \tilde{f}(x)|} \propto (t - t_\ast)^{(3-2\alpha)/4(\alpha-1)}.$$  \hspace{1cm} (6)

As follows from general considerations and is supported by direct numeric analysis [10], $\tilde{f}(x) \propto 1/x$ at $x \ll 1$, which means that the back wave creates a quasi-equilibrium distribution at $\varepsilon \ll \varepsilon_0(t)$ [with infinite at $t = t_\ast$ and ever decreasing afterwards temperature $\propto \varepsilon_0^{-\alpha}(t)$].

To estimate the parameter $A$ for a given initial conditions one extrapolates the solution (3) to a region of energies $\sim \varepsilon_{\text{init}}$, where the particles were initially concentrated with typical occupation numbers $n_{\varepsilon_{\text{init}}}$. This immediately yields $A \sim n_{\varepsilon_{\text{init}}} \varepsilon_{\text{init}}^{-\alpha}$.

### III. COHERENT REGIME

Strictly speaking, evolution in a kinetic regime does not lead to the ordering. It is seen from the fact that the description in terms of kinetic equation is associated with the random phase approximation (RPA) and thus valid only when the phases of $a_\nu$'s are practically uncorrelated. In such a state even local order (quasicondensate) is absent. Quasicondensate implies a strong change of the correlation properties as compared to the RPA state (3). It occurs in the regime of strong turbulence (so-called coherent regime), when typical time of evolutoion is comparable to the time of oscillation of the phases of relevant $a_\nu$'s. The essence of the process of the quasicondensate formation is the transformation of the strong turbulence into the state known as superfluid turbulence.

The degrees of freedom associated with the quasicondensate are the same as in a genuine condensate. These are phonons and topological defects (vortex lines). That is quasicondensate can be viewed as a condensate with (i) a tangle of vortex lines and (ii) strongly non-equilibrium distribution of long-wave phonons implying strong fluctuations of the phase of the quasicondensate part $\psi_\eta$ of the field $\psi$ at large distances.

Given the solution (3) of the kinetic equation, one readily estimates where and when the coherent regime sets in, and what is the typical density of the quasicondensate upon its formation. The characteristic time of evolution at the energy scale $\varepsilon$ is the collision time $\tau_{\text{coll}}^{-1}(\varepsilon)$, which is $\varepsilon^{-3/2}$ at the scale $\varepsilon_{\text{init}}$. The distribution $n_\varepsilon \sim A\varepsilon^{-\alpha}$ at the scale $\varepsilon_{\text{coh}}$ is formed at the time $t_{\text{coh}}$ obeying an obvious relation $\varepsilon_0(t = t_{\text{coh}} - t_\ast) \sim \varepsilon_{\text{coh}}$. Hence, $t_{\text{coh}}$ estimates the time moment when the coherent regime sets in. The time interval $[t_\ast - t_{\text{coh}}] \varepsilon_{\text{coh}}^{-1} \ll t_\ast$ is a typical time of the process of quasicondensate formation (in the strong turbulent regime all characteristic times and distances scale with $\varepsilon_{\text{coh}}^{-1}$ and $(2m\varepsilon_{\text{coh}})^{-1/2}$, correspondingly). The initial quasicondensate density $\eta_{\text{init}}$ is the density corresponding to the harmonics $\varepsilon \sim \varepsilon_{\text{coh}}$. It obeys an obvious relation $\eta_{\text{init}} U \sim \varepsilon_{\text{coh}}$, in accordance with the fact that in strong turbulent regime kinetic and potential energies are of the same order. The initial spacing between the vortex lines in the quasicondensate scales as $(2m\varepsilon_{\text{coh}})^{-1/2}$.

The coherent regime and the back wave are practically independent processes, with a reservation that the coherent part of the field is being pumped with particles from the high-energy region. This pumping, however, does not affect the character of the coherent evolution.

Relaxation of the quasicondensate towards genuine condensate goes in two directions: (i) relaxation of the vortex tangle [that is relaxation of the superfluid turbulence] and (ii) relaxation of the long-wave phonons. Both processes require a macroscopically large time (an analysis of this stage of evolution see in [8]).
IV. EXTERNAL POTENTIAL

In the experiments with trapped ultracold gases normally there takes place the Knudsen regime, when free path length of a particle with the energy $\varepsilon$, $l_{\text{free}}(\varepsilon)$, is much larger than the typical radius of the particle’s trajectory, $R_\varepsilon$. For definiteness we consider a parabolic trap with all the three frequencies of the same order $\omega_0$. So that $R_\varepsilon \sim \omega_0v(\varepsilon)$, $l(\varepsilon)$ is the typical velocity corresponding to the energy $\varepsilon$, and the condition $l_{\text{free}}(\varepsilon) \gg R_\varepsilon$ is equivalent to $\tau_{\text{coll}}(\varepsilon)\omega_0 \gg 1$.  

Knudsen regime is a very convenient starting point for analyzing kinetics in a potential. Almost in all qualitative aspects it corresponds to an isotropic homogeneous case, since the distribution of particles depends only on the two variables, $\varepsilon$ and $t$ (ergodic approximation). The main quantitative difference comes from the difference in the density of states, the scaling of the collision time remaining the same.

Initial picture of evolution is described by the self-similar wave (2)-(3) with $\alpha \approx 1.6$ [11,12]. The question then is: What happens when $t \rightarrow t_*$? The effect of the potential can be associated with two rather different reasons. The first reason is the essential discreteness of the low-lying energy levels, which drastically changes the kinetics when $\tau_{\text{coll}}(\varepsilon) < \Delta(\varepsilon)$, where $\Delta(\varepsilon)$ is the typical interlevel spacing. The second reason is the violation of the Knudsen regime at the head of the wave at some stage of evolution [because of the decreasing $\tau_{\text{coll}}(\varepsilon_0(t))$ with $t$].

Remarkably, the above-mentioned two circumstances arise always separately, and (apart a certain cross-over region) there is nothing in between. More specifically, as it immediately follows from the non-equality $\Delta(\varepsilon) < \omega_0$ and the fact that the relevant collision time $\tau_{\text{coll}}(\varepsilon_0(t))$ permanently decreases, if there occurs a break-down of Knudsen regime (in corresponding region of coordinate space with a typical size $R_{Kn}$ around the center of the potential), the discreteness of levels will never become relevant.

The case, when the discreteness of levels starts to act within the Knudsen regime, is rather transparent physically and is studied to a large extent both experimentally [13] and theoretically [11,12]. The evolution scenario in this case is as follows. When the wave reaches the scale where the level discreteness becomes relevant, its further propagation is suppressed (essentially discrete harmonics practically do not interact with each other) and the back wave is formed. At $\varepsilon < \varepsilon_0(t)$, the back wave generates quasi-equilibrium distribution with time-dependent permanently decreasing temperature $T(t)$ and permanently increasing number of particles. Condensation thus occurs in a quasi-equilibrium way, without the coherent stage (interaction between low-lying harmonics is negligible), and the whole process can be described within the kinetic approach [11,12].

We are mostly interested in the case, when at some time $t = t_{Kn}$ the Knudsen regime breaks down for energies $\varepsilon_{Kn} \sim \varepsilon_0(t = t_{Kn})$. From (2)-(3) we estimate $\varepsilon_{Kn} \sim [m^3U^2A^2/\omega_0]^{1/2(\alpha-1)}$. The size of corresponding spatial region is defined by $m\omega_0^2R_{Kn}^2 \sim \varepsilon_{Kn}$. We argue that within the region $r < R_{Kn}$ at $t > t_{Kn}$ the external potential becomes irrelevant at least until the quasicondensate is formed, so that the most important evolution stage basically does not differ from the homogeneous case. Indeed, it is quite natural that further evolution within the region $r < R_{Kn}$ will result in the formation of anti-Knudsen regime $l_{\text{free}}(\varepsilon) \ll R_{Kn}$ for $\varepsilon \ll \varepsilon_0(t_{Kn})$, because of increasing collision rate with increasing the occupations numbers. In the anti-Knudsen regime the evolution during the time period on the order of collision time is insensitive to the external potential (the criteria for the Knudsen regime and for the sensitivity to the potential within the collision time coincide). But this time is enough to form the wave (2)-(3) in the energy space (with the exponent $\alpha$ corresponding to the homogeneous case) and then to form quasicondensate. During the wave evolution in the energy space, the free-path length of the particles with $\varepsilon \sim \varepsilon_0(t)$ is getting progressively smaller, which renders the proposed scenario self-consistent. A minor deviation from the pure homogeneous picture is that now the moment $t_*$ depends on the distance from the center of the potential, so that the coherent regime first should start at $r = 0$ (the point of maximal initial density) and then gradually occupy all the anti-Knudsen region up to $r \sim R_{Kn}$. By this moment the quasicondensate is formed at $r \leq R_{Kn}$. In terms of the total number of particles, $N$, and the typical single-particle energy of the initial distribution in the potential, $\varepsilon_{in}$, the estimate for $R_{Kn}$ is: $R_{Kn} \sim [U^2N^2m^{5-2\alpha}\omega_0^{9-4\alpha}\varepsilon_{in}^{2(\alpha-3)}]^{1/4(\alpha-1)}$.

On the basis of the above discussion one can introduce the parameter

$$p = N^2\omega_0mU^2(\omega_0/\varepsilon_{in})^{6-2\alpha},$$

that determines which of the two regimes takes place under given initial conditions: the discrete-harmonic regime ($p \ll 1$), or the superfluid-turbulence one ($p \gg 1$).

For more details on the ordering kinetics in a trapped gas see [14].
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