Existence of Long-Range Order for Trapped Interacting Bosons

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We derive an inequality governing “long range” order for a localized Bose-condensed state, relating the condensate fraction at a given temperature with effective curvature radius of the condensate and total particle number. For the specific example of a one-dimensional, harmonically trapped dilute Bose condensate, it is shown that the inequality gives an explicit upper bound for the Thomas-Fermi condensate size which may be tested in current experiments.

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The classic Hohenberg theorem [1] employs the fact that in the thermodynamic limit of an infinite system of interacting particles of bare mass \( m \), the relation (\( h = k_B = 1 \))

\[
N_k \geq -\frac{1}{2} + \frac{m T}{k^2} n_0 \quad (1)
\]

for the occupation numbers \( N_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle \) of the plane wave states enumerated by \( k \neq 0 \) holds (the Bogoliubov \( 1/k^2 \) theorem [2]). The angled brackets here and in what follows indicate a thermal ensemble (quasi-)average [2]; \( n_0 \) and \( n \) are the condensate density and total density, respectively. The relation (1) entails that in one and two dimensions, a macroscopic occupation of a single state, the condensate, is impossible: The inequality leads to a contradiction in dimension \( D \leq 2 \) due to the (infrared) divergence of the wave vector space integral of (1), which determines the number density of non-condensate atoms. Physically, long range thermal fluctuations destroy the coherence expressed by the existence of the condensate.

The question of the applicability of the Hohenberg theorem to systems displaying long range order has renewed interest for trapped Bose-condensed vapors of reduced dimensionality, which can now be realized using various techniques [3, 4, 5, 6]. In these systems, it is possible to investigate in a controlled manner the influence of finite extension in different spatial directions on the existence of a condensate, i.e., a macroscopically occupied single state created by \( \hat{b}_0^\dagger \). For the non-interacting case, it is not difficult to show that there can exist a macroscopic occupation of one or several states in a Bose-condensed, trapped vapor of any dimension, as long as particle numbers remain finite, simply by evaluating the Bose-Einstein sums for the occupation numbers (see, e.g., [5]). The difficulty comes in when interaction is turned on. An interacting gas has a behavior increasingly different from the ideal gas the lower the dimension of the system [6, 7]. Furthermore, the classification of excited non-condensate states by plane waves is not the suitable one in a trapped gas: The condensation, in the limit of large total particle number \( N \), takes place primarily into a single particle state in co-ordinate space [8], and condensate and total densities have (in principle arbitrary) spatial dependence, \( n_0 \rightarrow n_0(r), n \rightarrow n(r) \). While a recent proof by Lieb and Seiringer shows that ground state condensation is, in the thermodynamic limit, 100% into the state that minimizes the Gross-Pitaevskii energy functional in three as well as in two dimensions [9, 10], the question of the existence of a condensate for general energy functionals, at finite temperatures and, in particular, in the generic one-dimensional (1D) case remains open.

In what follows, we will take account of the phenomenon of spatially localized Bose-Einstein condensates, by deriving an inequality analogous to the integral of (1), with no explicit dependence on any Hamiltonian which has velocity independent interaction and trapping potentials. At a given finite temperature, the maximally allowed condensate fraction is related to an effective curvature radius of the condensate and the total particle number. The inequality thus allows for concrete statements on the limiting size of quantum coherent systems of reduced dimensionality, and their realizability for given condensate and total density distributions. As an application to a specific example, we consider a 1D harmonically trapped, dilute Bose-Einstein condensate, and it is shown that the relation leads to bounds on the parameters of a Thomas-Fermi cloud which may be verified in present experiments.

Our analysis is based upon the following decomposition of field and density operators into condensate and non-condensate parts:

\[
\hat{\Phi}(r) = \Phi_0(r) \hat{b}_0 + \delta \Phi(r)
\]
\[
\hat{\rho}(r) = |\Phi_0(r)|^2 \hat{b}_0^\dagger \hat{b}_0 + \delta \rho(r)
\]
\[
\delta \hat{\rho}(r) = \Phi_0^\dagger(r) \hat{b}_0^\dagger \delta \Phi(r) + \text{h.c.} + \delta \Phi^\dagger(r) \delta \Phi(r),
\]

where \( \Phi_0(r) \) is the single particle condensate wave function (normalized to unity) and \( N_0 |\Phi_0(r)|^2 \) is the condensate density. The commutation relation

\[
\left[ \delta \Phi(r), \delta \Phi^\dagger(r') \right] = \delta(r - r') - \Phi_0(r) \Phi_0^\dagger(r'),
\]

is obtained from the canonical commutation relations for the quantum fields \( \Phi(r), \Phi^\dagger(r) \). As a consequence of this
commutator, the mixed response (the “anomalous” commutator) is taking the nonlocal form
\[
\left\langle \left[ \hat{\rho}(r), \delta \hat{\Phi} (r') \right] \right\rangle = \sqrt{N_0} \Phi_0 (r) \left[ \Phi_0^\dagger (r) \Phi_0 (r') - \delta (r - r') \right].
\] (4)

Here, after carrying out the commutator, \( \langle b_0 \rangle = \sqrt{N_0} = \langle \hat{b}_0 \rangle \) has been used, where this assignment is valid to \( O(1/\sqrt{N_0}) \). The first term in the brackets on the RHS is due to the second term in the commutator (3). It vanishes if one takes the Bogoliubov prescription that \( \hat{b}_0 \) and \( \hat{b}_0^\dagger \) be replaced by c-numbers. It is a well-established fact that this (standard) Bogoliubov approach violates particle number conservation \( [13] \), and it becomes apparent below that neglecting the second term on the RHS of (3) would lead to numerically strongly different predictions for the allowed condensate fraction.

We now make use of this form of the mixed response in the Bogoliubov inequality \( [4] \), which reads
\[
\frac{1}{2} \left\langle \left\{ \hat{A}, \hat{A}^\dagger \right\} \right\rangle \geq \frac{T}{\langle [\hat{C}, \hat{H}], \hat{C}^\dagger \rangle} \left( \left\langle [\hat{C}, \hat{H}], \hat{C}^\dagger \right\rangle \right)^2
\] (5)
for any two operators \( \hat{A} \) and \( \hat{C} \), where \( T \) is the temperature. It is valid for any many-body quantum system, for which the indicated thermal (quasi-)averages are well-defined. We choose the operators in relation (3) to be the smeared excitation and total density operators
\[
\hat{A} = \int d^D r f(r) \delta \hat{\Phi} (r),
\] (6)
\[
\hat{C} = \int d^D r g(r) \hat{\rho} (r),
\] (7)
where \( f(r) \) and \( g(r) \) are complex regularization kernels.

Next we derive a sum rule for the denominator on the RHS of (3), analogous to the \( f \)-sum rule
\[
\int_{-\infty}^{\infty} d\omega \omega S(k, \omega) = Nk^2/m \text{ for the dynamic structure factor} \ [14], \text{ but in co-ordinate space. Using that}
\]
\[
\left\langle \left[ \left[ \hat{\rho} (r), \hat{H} (r) \right], \delta \hat{\rho} (r') \right] \right\rangle = -i \left\langle \left[ \left[ \nabla_r \cdot \hat{j} (r), \hat{\rho} (r') \right] \right\rangle \right\rangle
\]
\[
= \frac{1}{2m} \left\langle \delta (r - r') \left[ \hat{\Phi} (r) \Delta_r \hat{\Phi} (r) + \text{h.c.} \right] - \Delta_r \delta (r - r') \left[ \hat{\Phi} (r) \hat{\Phi} (r) + \text{h.c.} \right] \right\rangle,
\] (8)
we obtain that the double commutator equals
\[
\left\langle \left[ \left[ \hat{C}, \hat{H} \right], \hat{C}^\dagger \right] \right\rangle = \frac{1}{m} \int d^D r \left( -\Delta_r g(r) \right) g^*(r) n(r),
\] (9)
where \( n(r) = \langle \hat{n} (r) \rangle = \langle \hat{\Phi}^\dagger (r) \hat{\Phi} (r) \rangle \). Here, we used the continuity equation for the current density operator \( \hat{j} = \left[ \hat{\Phi} \delta \hat{\Phi} \right] / 2im \), together with the Heisenberg equation of motion for \( \hat{\rho} \): \( [\hat{\rho}, \hat{H}] = i \partial_r \hat{\rho} = -i \nabla \cdot \hat{j} \), this last relation being valid for a Hamiltonian with no explicit velocity dependence in the interaction and external potentials \( [14] \).

We normalize the kernel \( f(r) \) to unity, i.e., \( \int d^D r |f(r)|^2 = 1 \). The left hand side of the Bogoliubov inequality (3) is then bounded from above, using the Cauchy-Schwarz inequality, as follows
\[
\frac{1}{2} \int d^D r \int d^D r' f(r) f^*(r') \left\langle \left\{ \delta \hat{\Phi} (r), \delta \hat{\Phi}^\dagger (r') \right\} \right\rangle \leq \int d^D r' \left\langle \delta \hat{\Phi} (r') \delta \hat{\Phi}^\dagger (r') \right\rangle + \frac{a}{2}
\]
\[
= N - N_0 + \frac{a}{2},
\] (10)
where the quantity \( a \leq 1 \) is given by \( a = 1 - \int d^D r \int d^D r' f(r) f^*(r') \Phi_0(r) \Phi_0^\dagger (r') \), and where \( N - N_0 = \int d^D r \delta \hat{\rho} (r) = \int d^D r \delta \hat{\Phi} (r) \delta \hat{\Phi} (r) > 0 \) is the excited number of particles.

Using the anomalous commutator (1), the Bogoliubov inequality (2) thus may be written in the following form:

\[
N - N_0 \geq -\frac{a}{2} + mT N_0 \left[ \int d^D r g(r) f(r) \Phi_0 (r) - \int d^D r \int d^D r' g(r) f(r') |\Phi_0 (r)|^2 |\Phi_0 (r')|^2 \right] /
\int d^D r \left( -\Delta_r g(r) \right) g^*(r) n(r).
\] (11)

It is important to recognize that the above relation is explicitly independent of the form of the excitation spectrum of the system, due to the relation (3). In particular, the strength of the interaction enters only implicitly in the form of the condensate wave function and total density distribution. This is in contrast to previous considerations on “long range” order in Bose-Einstein condensates, employing correlation functions \( [10] [13] \), where use was made of the excitation spectrum of the system, with Bogoliubov-type or WKB approximations.

Now choose the kernels to have the particular form
\[
f_k (r) = \begin{cases} \Omega_0^{-1/2} \exp[i k \cdot r] & (r \in D_0) \\ 0 & (r \notin D_0) \end{cases}
\]
\[ g(r) = \begin{cases} \Phi_0^*(r) & (r \in D_0) \\ 0 & (r \not\in D_0) \end{cases} \tag{12} \]

where \( \Omega_0 \) is the volume of the domain \( D_0 \) in which \( \Phi_0 \) has finite support. Hence \( |g|^2 \) is also, automatically, normalized to unity, \( \int_{D_0} d^D r |g|^2 = \int_{D_0} d^D r |\Phi_0|^2 = 1 \).

The Fourier transforms of single particle condensate density and wave function are defined to be \( \tilde{\rho}_0(k) = \int d^D r |\Phi_0(r)|^2 \exp[ik \cdot r] \) and \( \tilde{\Phi}_0(k) = \int d^D r \Phi_0(r) \exp[ik \cdot r] \).

We define the effective radius of curvature of the condensate to be

\[ R_c = \sqrt{\frac{N}{\Omega_0} \left( \int_{D_0} d^D r \Phi_0(r) \left[ -\Delta_r \Phi_0^*(r) \right] n(r) \right)^{-1/2}} \tag{14} \]

According to the above formula, \( R_c \) is obtained by weighing a quantity proportional to the kinetic energy density of the condensate with \( n(r)/(N/\Omega_0) \), i.e., the local density relative to the average density, and finally integrating over the domain \( D_0 \). Using this definition, relation (13) reads

\[ \frac{1 - F}{F} \geq \frac{1}{N \lambda_{\text{dB}}^2} C(k) - \frac{1}{2N_0} \left( 1 - |\tilde{\Phi}_0(k)|^2/\Omega_0 \right) \tag{15} \]

where the functional \( C(k) \) is given by

\[ C(k) = \left| \tilde{\rho}_0(k) - \tilde{\Phi}_0(k) \int_{D_0} d^D r \Phi_0^*(r) |\Phi_0(r)|^2 \right|^2 \tag{16} \]

and the condensate fraction \( F = N_0/N; \) the de Broglie thermal wavelength \( \lambda_{\text{dB}} = \sqrt{2\pi/mT} \). We stress that the value of \( C(k) \) is strongly reduced as a consequence of the commutation relation (3), which causes the second term under the square root in (14).

The relation (14) implies that for temperatures close to zero, such that \( F R_c^2/\lambda_{\text{dB}}^2 \) remains large (in which case the second term in (14) is negligible), the approach of \( NC^{-1}(1 - F) = C^{-1}(N - N_0) \propto T^a \) to zero with a power law has to fulfill \( a \leq 1 \) for complete Bose-Einstein condensation into a localized single state \( \Phi_0(r) \) to be possible. This statement holds for arbitrary strength and form of the interaction, in any spatial dimension.

The above relations (3) and (13) are general. The strongest result, i.e., constraint on the system parameters we may expect for a 1D system, in analogy to the original Hohenberg theorem (the \( 1/k \) infrared divergence of the integral of (1) in one dimension). To demonstrate the meaning of the relation (3) explicitly, we thus now proceed by considering the example of axially symmetric, harmonically trapped gases in one dimension, in the currently experimentally accessible Thomas-Fermi limit.

Consider the Thomas-Fermi wave function

\[ \Phi_0(z) = \sqrt{\frac{n_{TF}^2}{N}} \left( 1 - \frac{z^2}{Z_{TF}^2} \right)^{1/2} \tag{17} \]

This mean-field form of \( \Phi_0 \) is valid if the 1D scattering length fulfills the strong coupling condition \( n_0(a_{1D}) \gg 1 \), and the Thomas-Fermi parameters are \( Z_{TF} = (3N \bar{d}_L^2/a_{1D})^{1/3} \), \( n_{TF}^2 = [(9/64)N^2 a_{1D}/\bar{d}_L^3]^{1/3} \), the quantities \( d_{L,z} = (m \omega_{L,z})^{-1/2} \) are the harmonic oscillator lengths. In the quasi-3D scattering limit, which has transverse length scale \( a_{1D} \gg a_s \), the 1D scattering length is given by \( a_{1D} = -a_s/(2a_s) \), with \( C = 1.4603 \). We neglect the difference between \( n(r) \) and \( N |\Phi_0(r)|^2 \), i.e., take the limit of both sides of (13) to linear order in \( 1 - F \). Evaluating the elementary integrals involved, we obtain that \( (x \equiv k Z_{TF}) \)

\[ C(x) = \frac{3}{x^2} \left( \sin x - \cos x \right) - \frac{27 \pi^2 J_1(x)}{128 x} \tag{18} \]

where \( J_1(x) \) is a Bessel function of the first kind. We see from Fig. 4 that the function \( C \) is strongly peaked at its global maximum \( k_m \approx 3.7 Z_{TF}^{-1} \lambda_{\text{dB}} \). Using the second term on the RHS of (3), we obtain at \( k = k_m \)

\[ \frac{Z_{TF}}{\lambda_{dB}} \leq 6.0 \sqrt{N - N_0} \tag{19} \]

We compare the above relation with the experiment on a 1D \( ^{23}\text{Na} \) condensate in [3], where the (relatively moderate) parameters were \( a_s = 2.8 \times 10^{-3} \text{\mu m} \), \( d_z = 11.2 \text{\mu m} \) (\( \omega_z/2\pi = 3.5 \text{Hz} \)), \( d_{L,z} = 1.15 \text{\mu m} \), and \( N \sim 1.5 \times 10^5 \),
which result in $Z_{TF} \approx 150 \mu m$. Inequality (14) becomes $Z_{TF}/\lambda_{AB} \lesssim 7.3 \times 10^2 \sqrt{1-F}$. Temperatures in this experiment have been of the order $T \sim O(100\text{mK})$ [7], which gives $\lambda_{AB} \approx 1 \mu m$ and $Z_{TF}/\lambda_{AB} \simeq 1.5 \times 10^2$. The parameters of [3] are thus consistent with (19), provided $F$ is not too close to unity [18]. Note that (19) would be inconsistent with the parameters in that experiment, were it not for the commutation relation (3), due to imposing the canonical commutation relations for the total quantum field. Neglecting the second term on the RHS of [3] leads to a decrease of the RHS of (19) by about one order of magnitude. In this sense, particle number conservation, which is violated by the standard Bogoliubov prescription, is necessary for the condensate to exist [19].

A further decrease of the aspect ratio $\omega_z/\omega_\perp = d_z^2/d_\perp^2$ down to values of order $10^{-3}$ and lower is achievable, e.g., in optical lattices [8], so that the condition (19) on the trap parameters should be experimentally verifiable within present technology. When (19) ceases to be fulfilled, the system has to enter into a new (non-Thomas-Fermi) state. For very low densities, a “Tonks gas” (1D gas of impenetrable particles) may be formed, which has no condensate [13] [14] [20]. Another possibility is a condensate consisting of (overlapping) phase coherent droplets [21], resulting in a reduced value of $R_c$.

The primary result of the present investigation, inequality (13), holds under the generic conditions that the Bogoliubov inequality (3) is valid and that the potentials in the Hamiltonian are independent of particle velocities. It is, furthermore, to be emphasized that the application of (13) is by no means limited to (real) ground state forms of $\Phi_0$. It is also possible to employ this relation to examine existence conditions for excited state condensates with complex $\Phi_0$, like single vortices or vortex lattices. While (13) certainly cannot guarantee the existence of a given $\{N_0, \Phi_0(r), n(r)\}$ state, it can rule out models for trapped Bose-condensed gases in various spatial dimensions which are inconsistent with the Bogoliubov inequality (3).

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