Proof of Bose-Einstein Condensation for Dilute Trapped Gases

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The ground state of bosonic atoms in a trap has been shown experimentally to display Bose-Einstein condensation (BEC). We prove this fact theoretically for bosons with two-body repulsive interaction potentials in the dilute limit, starting from the basic Schrödinger equation; the condensation is 100% into the state that minimizes the Gross-Pitaevskii energy functional. This is the first rigorous proof of BEC in a physically realistic, continuum model.

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It is gratifying to see the experimental realization, in traps, of the long-predicted Bose-Einstein condensation (BEC) of gases. From the theoretical point of view, however, a rigorous demonstration of this phenomenon – starting from the many-body Hamiltonian of interacting particles – has not yet been achieved. In this letter we provide such a rigorous justification for the ground state of 2D or 3D bosons in a trap with repulsive pair potentials, and in the well-defined limit (described below) in which the Gross-Pitaevskii (GP) formula is applicable. It is the first proof of BEC for interacting particles in a continuum (as distinct from lattice) model and in a physically realistic situation.

The difficulty of the problem comes from the fact that BEC is not a consequence of energy considerations alone. The correctness of Bogolubov’s formula for the ground state energy per particle, $e_0(\rho)$, of bosons at low density $\rho$, namely $e_0(\rho) = 2\pi h^2 \rho a/m$ (with $m =$ particle mass and $a =$ scattering length of the pair potential) shows only that ‘condensation’ exists on local length scales. The same is true in 2D, with Schick’s formula $e_0(\rho) = 2\pi h^2 \rho/(m \ln(\rho a^2))$. Although it is convenient to assume BEC in the derivation of $e_0(\rho)$, these formulas for $e_0(\rho)$ do not prove BEC. Indeed, in 1D the assumption of BEC leads to a correct formula for $e_0(\rho)$, but there is, presumably, no BEC in 1D ground states.

The results just mentioned are for homogeneous gases in the thermodynamic limit. For traps, the GP formula is exact in the limit, and one expects BEC into the GP function (instead of into the constant, or zero momentum, function appropriate for the homogeneous gas). This is proved in Theorem 1. In the homogeneous case the BEC is not 100%, even in the ground state. There is always some ‘depletion’. In contrast, BEC in the GP limit is 100% because the $N \rightarrow \infty$ limit is different.

In the homogeneous case one fixes $a > 0$ and takes $N \rightarrow \infty$ with $\rho = N/volume$ fixed. For the GP limit one fixes the external trap potential $V(\mathbf{r})$ and fixes $Na$, the ‘effective coupling constant’, as $N \rightarrow \infty$. A particular, academic example of the trap is $V(\mathbf{r}) = 0$ for $\mathbf{r}$ inside a unit cube and $V(\mathbf{r}) = \infty$ otherwise. By scaling, one can relate this special case to the homogeneous case and thereby compare the two limits; one sees that the homogeneous case corresponds, mathematically, to the trap case with this special $V$, but with $Na^3 = \rho a^3$ fixed as $N \rightarrow \infty$. Thus, BEC in the trap case is the easier of the two, reflecting the incompleteness of BEC in the homogeneous case. The lack of depletion in the GP limit is consistent with $\rho a^3 \rightarrow 0$ and with Bogolubov theory.

We now describe the setting more precisely. We concentrate on the 3D case, and comment on the generalization to 2D at the end of this letter. The Hamiltonian for $N$ identical bosons in a trap potential $V$, interacting via a pair potential $v$, is

$$H = \sum_{i=1}^{N} (-\Delta_i + V(\mathbf{r}_i)) + \sum_{1 \leq i < j \leq N} v(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

It acts on symmetric functions of $N$ variables $\mathbf{r}_i \in \mathbb{R}^3$. Units in which $\hbar^2/2m = 1$ are used. We assume the trap potential $V$ to be a locally bounded function, that tends to infinity as $|\mathbf{r}| \rightarrow \infty$. The interaction potential $v$ is assumed to be nonnegative, spherically symmetric, and have a finite scattering length $a$. (For the definition of scattering length, see 2, 3 or 4.) Note that we do not demand $v$ to be locally integrable; it is allowed to have a hard core, which forces the wave functions to vanish whenever two particles are close together. In the following, we want to let $a$ vary with $N$, and we do this by scaling, i.e., we write $v(\mathbf{r}) = v_1(r/a)/a^2$, where $v_1$ has scattering length 1, and keep $v_1$ fixed when varying $a$.

The Gross-Pitaevskii functional is given by

$$\mathcal{E}^{\text{GP}}[\phi] = \int \left( |\nabla \phi(\mathbf{r})|^2 + V(\mathbf{r})|\phi(\mathbf{r})|^2 + g|\phi(\mathbf{r})|^4 \right) \, d^3\mathbf{r}.$$

The parameter $g$ is related to the scattering length of the interaction potential appearing in (1) via

$$g = 4\pi Na. \quad (2)$$

We denote by $\phi^{\text{GP}}$ the minimizer of $\mathcal{E}^{\text{GP}}$ under the normalization condition $\int |\phi|^2 = 1$. Existence, uniqueness, and some regularity properties of $\phi^{\text{GP}}$ were proved in the appendix of 6. In particular, $\phi^{\text{GP}}$ is continuously differentiable and strictly positive. Of course $\phi^{\text{GP}}$ depends on...
$g$, but we omit this dependence for simplicity of notation. For use later, we define the projector

$$
P_{GP} = |\phi_{GP}\rangle\langle\phi_{GP}| .
$$

It was shown in [3] (see also Theorem 2 below) that, for each fixed $g$, the minimization of the GP functional correctly reproduces the large $N$ asymptotics of the ground state energy and density of $H$ – but no assertion about BEC in this limit was made in [3].

BEC in $\Psi$, the (nonnegative and normalized) ground state of $H$, refers to the reduced one-particle density matrix

$$
\gamma(r,r') = N \int \Psi(r,X)\Psi(r',X)dX ,
$$

where $X = (r_2,\ldots,r_N)$ and $dX = \prod_{j=2}^N d^3r_j$.

Complete (or 100%) BEC is defined to be the property that $\hat{\gamma}$ becomes a simple product $f(r)f(r')$ as $N \to \infty$, in which case $f$ is called the condensate wave function. In the GP limit, i.e., $N \to \infty$ with $g = 4\pi Na$, we can show that this is the case, and the condensate wave function is, in fact, the GP minimizer $\phi_{GP}$.

**THEOREM 1 (Bose-Einstein Condensation).** For each fixed $g$

$$
\lim_{N \to \infty} \frac{1}{N} \gamma(r,r') = \phi_{GP}(r)\phi_{GP}(r') .
$$

Convergence is in the senses that $\text{Trace} \left| \frac{1}{N} \gamma - P_{GP} \right| \to 0$ and $\int \left( \frac{1}{2N} \gamma(r,r') - \phi_{GP}(r)\phi_{GP}(r') \right)^2 d^3r d^3r' \to 0$.

We remark that Theorem 1 implies that there is 100% condensation for all $n$-particle reduced density matrices of $\Psi$, i.e., they converge to the one-dimensional projector onto the corresponding $n$-fold product of $\phi_{GP}$. To see this, let $a^*, a$ denote the boson creation and annihilation operators for the state $\phi_{GP}$, and observe that

$$
1 \geq N^{-n} \langle \Psi | (a^*)^n a^n | \Psi \rangle \approx N^{-n} \langle \Psi | (a^*)^n a^n | \Psi \rangle \geq N^{-n} \langle \Psi | a^* a | \Psi \rangle^n \to 1 ,
$$

where the terms coming from the commutators $[a, a^*] = 1$ can be neglected since they are of lower order as $N \to \infty$. The last inequality follows from convexity.

Another corollary, important for the interpretation of experiments, concerns the momentum distribution of the ground state.

**COROLLARY 1 (Convergence of Momentum Distribution).** Let $\hat{\rho}(k) = \int \gamma(r,r') \exp[i k \cdot (r-r')] d^3r d^3r'$ denote the one-particle momentum density of $\Psi$. Then, for each fixed $g$,

$$
\lim_{N \to \infty} \frac{1}{N} \hat{\rho}(k) = |\hat{\phi}_{GP}(k)|^2
$$

in the sense that $\int \left| \frac{1}{N} \hat{\rho}(k) - |\hat{\phi}_{GP}(k)|^2 \right| d^3k \to 0$. Here, $\hat{\phi}_{GP}$ denotes the Fourier transform of $\phi_{GP}$.

**Proof.** If $F$ denotes the (unitary) operator ‘Fourier transform’ and if $\varphi$ is an arbitrary bounded function with bound $\|\varphi\|_\infty$, then

$$
\left| \frac{1}{N} \int \hat{\rho} \varphi - \int |\phi_{GP}|^2 \varphi \right| = \left| \text{Trace} \left[ F^\dagger (\gamma/N - P_{GP}) F \varphi \right] \right| 
$$

$$
\leq \|\varphi\|_\infty \text{Trace} |\gamma/N - P_{GP}| ,
$$

whence $\int \left| \hat{\rho} - |\phi_{GP}|^2 \right| \leq \text{Trace} |\gamma/N - P_{GP}|$, QED.

Before proving Theorem 1, let us state some prior results on which we shall build. Then we shall outline the proof and formulate two lemmas, which will allow us to prove Theorem 1. We conclude with the proof itself.

Denote by $E^{QM}(N,a)$ the ground state energy of $H$ and by $E^{GP}(g)$ the lowest energy of $\mathcal{E}^{GP}$ with $\|\phi\|^2 = 1$. The following Theorem 2 can be deduced from [3].

**THEOREM 2 (Asymptotics of Energy Components).** Let $\rho(r) = \gamma(r,r)$ denote the density of the ground state $H$. For fixed $g = 4\pi Na$,

$$
\lim_{N \to \infty} \frac{1}{N} E^{QM}(N,a) = E^{GP}(g) \quad (4a)
$$

and

$$
\lim_{N \to \infty} \frac{1}{N} \rho(r) = |\phi_{GP}(r)|^2 \quad (4b)
$$

in the same sense as in Corollary 1. Moreover, if $\varphi_1$ denotes the solution to the scattering equation for $v_1$ (under the boundary condition $\lim_{r_1 \to \infty} \varphi_1(r_1) = 1$) and $s = \int |\nabla \varphi_1|^2/4\pi$, then $0 < s \leq 1$ and

$$
\lim_{N \to \infty} \int \nabla r_1 \cdot \Psi(r_1,X) d^3r_1 dX
$$

$$
= \int \nabla \phi_{GP}(r) d^3r + gs \int |\phi_{GP}(r)|^4 d^3r , \quad (5a)
$$

$$
\lim_{N \to \infty} \int V(r_1) |\Psi|^2 d^3r_1 dX = \int V(r) |\phi_{GP}(r)|^2 d^3r , \quad (5b)
$$

$$
\lim_{N \to \infty} \frac{1}{2} \sum_{j=2}^N \int \varphi(r_1 - r_j) \Psi(r_1,X) d^3r_1 dX
$$

$$
= (1 - s) g \int |\phi_{GP}(r)|^4 d^3r . \quad (5c)
$$

Only [3] was proved in [6], but [3] follows, as noted in [8], by multiplying $V$ and $v$ by parameters and computing the variation of the energy with respect to them.

(technical note: The convergence in [3] was shown in [3] to be in the weak $L^1(\mathbb{R}^3)$ sense, but our result here implies strong convergence, in fact. The proof in Corollary 1, together with Theorem 1 itself, implies this.)

**Outline of Proof:** There are two essential ingredients in our proof of Theorem 1. The first is a proof that the part of the kinetic energy that is associated with the interaction $v$ (namely, the second term in (3b)) is mostly located in small balls surrounding each particle. More
precisely, these balls can be taken to have radius $N^{-7/17}$, which is much smaller than the mean-particle spacing $N^{-1/3}$. This allows us to conclude that the function of $r$ defined for each fixed value of $X$ by

$$f_X(r) = \frac{1}{\phi_{GP}(r)} \psi(r, X) \geq 0$$

has the property that $\nabla_r f_X(r)$ is almost zero outside the small balls centered at points of $X$.

The complement of the small balls has a large volume but it can be a weird set; it need not even be connected. Therefore, the smallness of $\nabla_r f_X(r)$ in this set does not guarantee that $f_X(r)$ is nearly constant (in $r$), or even that it is continuous. We need $f_X(r)$ to be nearly constant in order to conclude BEC. What saves the day is the total kinetic energy of $f_X(r)$ (including the balls) is not huge. The result that allows us to combine these two pieces of information in order to deduce the almost constancy of $f_X(r)$ is the generalized Poincaré inequality in Lemma 2. (End of Outline.)

Using the results of Theorem 2, partial integration and the GP equation (i.e., the variational equation for $\phi_{GP}$, see (3), Eq. (2.4)) we see that

$$\lim_{N \to \infty} \int |\phi_{GP}(r)|^2 |\nabla_r f_X(r)|^2 d^3 r \, dX = g s \int |\phi_{GP}|^4 d^3 r. \quad (7)$$

The following Lemma shows that to leading order all the energy in $\{0\}$ is concentrated in small balls.

**Lemma 1 (Localization of Energy).** For fixed $X$ let

$$\Omega_X = \left\{ r \in \mathbb{R}^3 \bigg| \min_{k \geq 2} |r - r_k| \geq N^{-7/17} \right\}. \quad (8)$$

Then

$$\lim_{N \to \infty} \int dX \int_{\Omega_X} d^3 r |\phi_{GP}(r)|^2 |\nabla_r f_X(r)|^2 = 0. \quad (9)$$

**Proof.** We shall show that, as $N \to \infty$,

$$\int dX \int_{\Omega_X} d^3 r |\phi_{GP}(r)|^2 |\nabla_r f_X(r)|^2$$

$$+ \frac{1}{2} \int dX \int d^3 r |\phi_{GP}(r)|^2 \sum_{k > 2} v(r - r_k)|f_X(r)|^2$$

$$- 2g \int dX \int d^3 r |\phi_{GP}(r)|^4 |f_X(r)|^2$$

$$\geq - g \int |\phi_{GP}(r)|^4 d^3 r - o(1),$$

which implies the assertion of the Lemma by virtue of (6) and the results of Theorem 2. Here, $\Omega_X^c$ is the complement of $\Omega_X$. The proof of (3) is actually just a detailed examination of the lower bounds to the energy derived in (3) and (4), and we use the methods in (3) and (4), just describing the differences from the case considered here.

Writing $f_X(r) = \Pi_{i \geq 2} \phi_{GP}(r_k) F(r, X)$ and using that $F$ is symmetric in the particle coordinates, we see that $[0]$ is equivalent to

$$\frac{1}{N} Q(F) \geq - g \int |\phi_{GP}|^4 - o(1), \quad (10)$$

where $Q$ is the quadratic form

$$Q(F) = \sum_{i=1}^N \int_{\Omega_i} |\nabla_i |^2 \prod_{k=1}^N |\phi_{GP}(r_k)|^2 d^3 r_k$$

$$+ \sum_{1 \leq i < j \leq N} \int \phi(r_i - r_j)|F|^2 \prod_{k=1}^N |\phi_{GP}(r_k)|^2 d^3 r_k$$

$$- 2g \sum_{i=1}^N |\phi_{GP}(r_i)|^2 |F|^2 \prod_{k=1}^N |\phi_{GP}(r_k)|^2 d^3 r_k, \quad (11)$$

with $\Omega_i^c = \{ (r_1, X) \in \mathbb{R}^{3N} | \min_{k \neq i} |r_i - r_k| \leq N^{-7/17} \}$. While (10) is not true for all conceivable $F$ satisfying the condition $\int |F|^2 \prod_{k=1}^N |\phi_{GP}(r_k)|^2 d^3 r_k = 1$, it is true for an $F$, such as ours, that has bounded kinetic energy $[4]$. Eqs. (4.11)–(4.12), (4.23)–(4.25), proved in [4], are similar to (10), (11) and almost establish (10), but there are two differences which we now explain.

(i) In our case, the kinetic energy of particle $i$ is restricted to the subset of $\mathbb{R}^{3N}$ in which $\min_{k \neq i} |r_i - r_k| \leq N^{-7/17}$. However, from the proof of the lower bound to the ground state energy of a homogeneous Bose gas derived in [1] (especially Lemma 1 and Eq. (26) there), which enters the calculations in (10), we see that only this part of the kinetic energy enters the proof of the lower bound — except for some additional piece with a relative magnitude $\varepsilon = O(N^{-2/17})$. In the notation of (10) the radius of the balls used in the application of Lemma 1 is chosen to be $R = aY^{-5/17}$, which, in the GP regime, is $R = O(N^{-7/17})$ since, for fixed $N$, $Y = O(a^2 N) = O(N^{-2})$. (See [1] for a fuller discussion about the choice of $R$.) The a-priori knowledge that the total kinetic energy is bounded by (11) tells us that the ‘additional piece’ which is $\varepsilon$ times the total kinetic energy, is truly $O(\varepsilon)$ and goes to zero as $N \to \infty$.

(ii) In (10) all integrals were restricted to some arbitrarily big, but finite box of size $R'$. However, the difference in the energy is easily estimated to be smaller than $2gN \times \max_r |\psi(r)|^2 |\phi_{GP}(r)|^2$, which, divided by $N$, is arbitrarily small, since $\phi_{GP}(r)$ decreases faster than exponentially at infinity (Lemma A.5).

Proceeding exactly as in (10) and taking the differences (i) and (ii) into account, we arrive at (10). QED

In the following, $K \subset \mathbb{R}^m$ denotes a bounded and connected set that is sufficiently nice so that the Poincaré-Sobolev inequality (see [10], Theorem 8.12) holds on $K$. In particular, this is the case if $K$ satisfies the cone property $[10]$ (e.g., if $K$ is a ball or a cube).

We introduce the general notation that $f \in L^p(K)$ if the norm $\|f\|_{L^p(K)} = \left[ \int_K |f(r)|^p d^m r \right]^{1/p}$ is finite.
LEMMA 2 (Generalized Poincaré Inequality). For $m \geq 2$ let $K \subset \mathbb{R}^m$ be as explained above, and let $h$ be a bounded function with $\int_K h = 1$. There exists a constant $C$ (depending only on $K$ and $h$) such that for all sets $\Omega \subset K$ and all $f \in H^1(\Omega)$ (i.e., $f \in L^2(\Omega)$ and $\nabla f \in L^2(\Omega)$) with $\int_K fh \, d^m r = 0$, the inequality

$$\int_\Omega |\nabla f(\mathbf{r})|^2 \, d^m r + \left(\frac{|\Omega|}{|K|}\right)^{2/m} \int_K |\nabla f(\mathbf{r})|^2 \, d^m r \leq \frac{1}{C} \int_K |f(\mathbf{r})|^2 \, d^m r$$

holds. Here $| \cdot |$ is the volume of a set, and $\Omega^c = K \setminus \Omega$.

Proof. Here $| \cdot |$ is the volume of a set, and $\Omega^c = K \setminus \Omega$. The usual Poincaré-Sobolev inequality on $\Omega$ (see [10], Theorem 8.12),

$$\|f\|_{L^2(K)}^2 \leq \tilde{C} \|\nabla f\|_{L^2(\Omega)}^2$$

$$\leq 2 \tilde{C} \left( \|\nabla f\|_{L^2(\Omega)}^2 + \|\nabla f\|_{L^2(\Omega)}^2 \right),$$

if $m \geq 2$ and $\int_K fh = 0$. Applying Hölder’s inequality

$$\|\nabla f\|_{L^2(\Omega)}^2 \leq \|\nabla f\|_{L^2(\Omega)} \Omega^{1/m}_{\Omega^c}$$

(and the analogue with $\Omega$ replaced by $\Omega^c$), we see that [12] holds with $C = 2|\Omega|^{2/m} \tilde{C}$.

The important point in Lemma 2 is that there is no restriction on $\Omega$ concerning regularity or connectivity.

Proof of Theorem 1. For some $R > 0$ let $K = \{ \mathbf{r} \in \mathbb{R}^3, |\mathbf{r}| \leq R \}$, and define

$$\langle f \rangle_K = \frac{1}{|K|} \int_K |\phi^{GP}(\mathbf{r})|^2 f(\mathbf{r}) \, d^3 r.$$