# Thermodynamic Limit and Proof of Condensation for Trapped Bosons

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We study condensation of trapped bosons in the limit when the number of particles tends to infinity. For the noninteracting gas we prove that there is no phase transition in any dimension, but in any dimension, at any temperature the system is 100% condensated into the one-particle ground state. In the case of an interacting gas we show that for a family of suitably scaled pair interactions, the Gross–Pitaevskii scaling included, a less-than-100% condensation into a single-particle eigenstate, which may depend on the interaction strength, persists at all temperatures.

**KEY WORDS:** Trapped Bose gas; Bose–Einstein condensation; scaled interactions.

## 1. INTRODUCTION

Bose–Einstein condensation (BEC) is one of the most fascinating collective phenomena occurring in Physics. More than three quarters of a century after its discovery, the condensation of a homogeneous Bose gas remains as enigmatic as ever, both experimentally and theoretically. Meanwhile, the experimental realization of condensation in trapped atomic gases has opened new perspectives for the theory as well. From the point of view of a mathematical treatment, the trapped and the homogeneous systems are quite different, mainly due to an energy gap above the—at most finitely degenerate—one-particle ground state of trapped Bose gases, implying that condensation occurs into a localized state. In the homogeneous gas the gap above the ground state vanishes in the thermodynamic limit. This makes condensation a subtle mathematical problem already in the noninteracting

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system, and an unsolved problem in the presence of any realistic interaction. The mathematical proof of condensation in a trap shows no comparable subtlety, although the gap endows the noninteracting gas with some peculiar properties, and condensation into a localized state makes some sort of scaling of the interaction unavoidable.

A recent important development in the theory of trapped gases was obtained by Lieb and Seiringer.[1] For a dilute interacting gas, in the limit when the particle number $N$ tends to infinity and the scattering length $a$ to zero in such a way that $Na$ is fixed, these authors proved a 100% BEC at zero temperature into the Hartree one-particle wavefunction.

The aim of the present paper is to study BEC in deep traps, both in the free and in the interacting cases. By a deep trap we mean a trap with an unbounded potential such that the corresponding one-body Hamiltonian $H^0$ has a pure point spectrum and $\exp(-\beta H^0)$ is trace class for any positive $\beta$. Such a trap gives no possibility of escape to the particle through thermal excitation. In Section 2 we prove a condition on the potential so that it gives rise to a deep trap.

In Section 3 we deel with the noninteracting gas in the limit when the particle number, $N$, tends to infinity. We show that asymptotically the total free energy is $N$ times the energy of the one-particle ground state, plus an $O(1)$ analytic function of $\beta$. There is no phase transition in any dimension $d \geqslant 1$, but the mean number of particles in excited states remains finite as $N$ goes to infinity, whatever be the temperature. So the density of the condensate is 1, condensation is 100% at all temperatures.

In Section 4 we use the results obtained for the noninteracting gas to prove the continuity of the phase diagram as a function of the interaction strength. In a first part, we define condensation into a one-particle state, and show that it is equivalent to having the largest eigenvalue of the one-particle reduced density matrix of order $N$. The second part of Section 4 contains the main result of the paper. Here we prove a theorem on Bose–Einstein condensation in an interacting gas. In particular, for a nonnegative interaction we obtain that, if the expectation value of the $N$-particle interaction energy taken with the ground state of the noninteracting gas is of the order of $N$, the occupation of at least one of the low-lying eigenstates of the one-particle Hamiltonian, which may depend on the interaction strength, is macroscopic. This holds true in any dimension and at any finite temperature. The result allows a finitely degenerate single-particle ground state (bosons with spin) and is nonperturbative in the sense that it does not depend on the size of the gap above the ground state. The occupation of the subspace of one-particle ground states tends to 100% with the vanishing interaction strength. In a corollary and in subsequent remarks we describe a family of nonnegative scaled interactions to which

the theorem applies. All these integrable pair interactions are weak, in the sense that their integral vanishes as $1/N$ with an increasing number of particles. Our examples include the Gross–Pitaevskii scaling limit in three dimensions and the opposite of Gross–Pitaevskii scaling in one dimension.

## 2. ONE-BODY HAMILTONIAN FOR DEEP TRAPS

The one-particle Hamiltonian we are going to use is

$$H^0 = -\frac{\hbar^2}{2m} \Delta + V \qquad (1)$$

on $L^2(\mathbb{R}^d)$, where the potential $V$ is chosen in such a way that $H^0$ has a pure point spectrum with discrete eigenvalues of finite multiplicity and $e^{-\beta H^0}$ is trace class, i.e., $\mathrm{tr}\, e^{-\beta H^0} < \infty$, for any $\beta > 0$. This condition ensures the finiteness of the one-particle free energy at any finite temperature $1/\beta$. We will refer to such a Hamiltonian as a deep trap. For the sake of simplicity, we shall also suppose that the ground state of $H^0$ is nondegenerate, so that the eigenvalues of $H^0$ are

$$\varepsilon_0 < \varepsilon_1 \leqslant \varepsilon_2 \leqslant \cdots. \qquad (2)$$

A large family of potentials corresponding to deep traps is characterized by the following proposition.

**Proposition 2.1.** Let $V: \mathbb{R}^d \to \mathbb{R}$ be bounded below and suppose that

$$\lim_{r \to \infty} \frac{\ln(r/r_0)}{V(\mathbf{r})} = 0 \qquad (3)$$

for some $r_0 > 0$. Then $\mathrm{tr}\, e^{-\beta H^0} < \infty$ for all $\beta > 0$.

Condition (3) is sharp in the sense that, as the proof will show it, a central or cubic potential which increases logarithmically leads to an exponentially increasing density of states and, therefore, a diverging trace for small positive $\beta$. Intuitively, the assertion of the proposition holds true because $\int \exp(-\beta V)\, d\mathbf{r} < \infty$ for any $\beta > 0$, but the connection is not immediate. We present two different proofs: The first uses the path integral representation of $\mathrm{tr}\, e^{-\beta H^0}$, while the second is based on a semiclassical estimation of the eigenvalues.

*First proof.*  Given $\beta > 0$, fix a $V_0 > d/\beta$. Let $V_m = \inf V(\mathbf{r}) > -\infty$. If (3) holds for an $r_0 > 0$ then it holds for any $r_0 > 0$. Choose $r_0$ so large that

$$V(\mathbf{r}) \geqslant V_m + V_0 \ln \frac{1}{2}\left(\frac{r}{r_0} + 1\right) \qquad \text{for all} \quad \mathbf{r} \in \mathbb{R}^d. \tag{4}$$

By the Feynman–Kac formula,[2]

$$\operatorname{tr} e^{-\beta H^0} = \int \langle \mathbf{r} | \, e^{-\beta H^0} \, | \mathbf{r} \rangle \, d\mathbf{r} = \int P_{00}^\beta(d\omega) \int e^{-\int_0^\beta V(\mathbf{r} + \omega(s))\, ds}\, d\mathbf{r}. \tag{5}$$

The first integral in the right member goes over (continuous) paths $\omega$ in $\mathbb{R}^d$ such that $\omega(0) = \omega(\beta) = 0$. $P_{xy}^\beta(d\omega)$ is the conditional Wiener measure, generated by $-\frac{\hbar^2}{2m}\varDelta$, for the time interval $[0, \beta]$, defined on sets of paths with $\omega(0) = \mathbf{x}$ and $\omega(\beta) = \mathbf{y}$. In Eq. (5) we have made use of the translation invariance of $P^\beta$. Let

$$\|\omega\|_\beta = \sup_{0 \leqslant s \leqslant \beta} |\omega(s)|. \tag{6}$$

The integral over $\mathbf{r}$ can be split in two parts. First,

$$\int_{r < 2\|\omega\|_\beta} e^{-\int_0^\beta V(\mathbf{r} + \omega(s))\, ds}\, d\mathbf{r} \leqslant e^{-\beta V_m} v_d (2\|\omega\|_\beta)^d \tag{7}$$

where $v_d$ is the volume of the $d$-dimensional unit ball. For $r > 2\|\omega\|_\beta$, we use (4) to obtain

$$V(\mathbf{r} + \omega(s)) \geqslant V_m + V_0 \ln \frac{r + 2r_0}{4r_0}. \tag{8}$$

After some algebra, this yields

$$\int_{r > 2\|\omega\|_\beta} e^{-\int_0^\beta V(\mathbf{r} + \omega(s))\, ds}\, d\mathbf{r} \leqslant \frac{e^{-\beta(V_m - V_0 \ln 2)} s_d}{\beta V_0 - d} (2r_0)^d. \tag{9}$$

Here $s_d$ is the surface area of the unit sphere in $\mathbb{R}^d$. Putting the two parts together,

$$\operatorname{tr} e^{-\beta H^0} \leqslant \frac{e^{-\beta(V_m - V_0 \ln 2)} s_d}{\beta V_0 - d} \left(\frac{2r_0}{\lambda_\beta}\right)^d + e^{-\beta V_m} v_d 2^d \int P_{00}^\beta(d\omega)(\|\omega\|_\beta)^d, \tag{10}$$

where we have substituted

$$\int P_{00}^{\beta}(\mathrm{d}\omega) = \langle 0| \, e^{\frac{\beta\hbar^2}{2m}\Delta} \, |0\rangle = \lambda_{\beta}^{-d}, \tag{11}$$

$\lambda_{\beta} = \hbar \sqrt{2\pi\beta/m}$ being the thermal de Broglie wave length. The second term on the right-hand side of (10) is finite: actually, every moment of the conditional Wiener measure is finite. Indeed, from the estimate (see Eqs. (1.14) and (1.31) of ref. 2)

$$P_{00}^{\beta}(\|\omega\|_{\beta} > 4\varepsilon) \leqslant \frac{2^{2+d/2}}{\lambda_{\beta}^d} \, (m_d + n_d(\varepsilon/\lambda_{\beta})^{d-1}) \, e^{-\pi\varepsilon^2/4\lambda_{\beta}^2} \tag{12}$$

where $m_d$ and $n_d$ depend only on the dimension $d$,

$$\int P_{00}^{\beta}(\mathrm{d}\omega)(\|\omega\|_{\beta})^k \leqslant \frac{2^{2+d/2}}{\lambda_{\beta}^d} \sum_{n=0}^{\infty} (n+1)^k \, (m_d + n_d(n/4\lambda_{\beta})^{d-1}) \, e^{-\pi n^2/64\lambda_{\beta}^2} < \infty. \tag{13}$$

This concludes the first proof.

*Second proof.* We start, as before, by fixing $\beta > 0$ and a $V_0 > d/\beta$. For the sake of convenience, now we choose $r_0$ so that

$$V(\mathbf{r}) \geqslant V_m + V_0 \ln \frac{1}{2}\left(\frac{r}{\sqrt{d}\, r_0} + 1\right) \qquad \text{for all} \quad \mathbf{r} \in \mathbb{R}^d. \tag{14}$$

The expression in the right member can still be bounded from below, due to the concavity of the square-root and the logarithm. With the notation $\mathbf{r} = (x_1,..., x_d)$, we find

$$V(\mathbf{r}) \geqslant V_m - V_0 \ln 2 + \frac{V_0}{d} \sum_{i=1}^{d} \ln\left(\frac{|x_i|}{r_0} + 1\right). \tag{15}$$

Let

$$h^0 = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{V_0}{d} \ln\left(\frac{|x|}{r_0} + 1\right). \tag{16}$$

Then

$$H^0 \geqslant V_m - V_0 \ln 2 + \sum_{i=1}^{d} h^0(i), \tag{17}$$

$h^0(i)$ acting on functions of $x_i$, and

$$\text{tr } e^{-\beta H^0} \leqslant e^{-\beta(V_m - V_0 \ln 2)}(\text{tr } e^{-\beta h^0})^d. \tag{18}$$

Let $\lambda_n$, $n \geqslant 0$, be the eigenvalues of $h^0$ in increasing order. From Theorem 7.4 of ref. 3, in the case of a logarithmic potential, it follows that any $\lambda \in [\lambda_{n-1}, \lambda_n]$ satisfies an equation of the form

$$\frac{\pi\hbar}{2}\left(n+\frac{1}{2}\right) = \int_0^X \sqrt{2m(\lambda - v(x))}\, dx + O(\lambda) \tag{19}$$

where $X$ is defined by $v(X) = \lambda$. Dropping $O(\lambda)$, the solution is the $n$th semiclassical eigenvalue according to the Bohr–Sommerfeld quantization. For the true $n$th eigenvalue equation (19) yields, after substituting $v(x) = (V_0/d)\ln(|x|/r_0 + 1)$,

$$\lambda_n = \frac{V_0}{d}\ln\left(n+\frac{1}{2}\right) + O(\ln\ln(n+3)), \qquad n = 0, 1, 2,\ldots. \tag{20}$$

So with a suitably chosen $c > 0$ we obtain the bound

$$\text{tr } e^{-\beta h^0} = \sum_{n=0}^{\infty} e^{-\beta\lambda_n} \leqslant \sum_{n=0}^{\infty} \frac{[\ln(n+3)]^{\beta c}}{(n+1/2)^{\beta V_0/d}} < \infty \tag{21}$$

which concludes the proof.

Observe that for $h^0$ and, thus, for the Hamiltonian $\sum_{i=1}^d h^0(i)$ the density of states can be inferred from Eq. (20), and shows an exponential growth with the energy. This is origin of the divergence of the trace for small $\beta$ in the case of logarithmically increasing potentials.

In the forthcoming proof of BEC at positive temperatures in interacting Bose gases, we shall make use of the following estimate.

**Proposition 2.2.** Let $e^{-\beta H^0}$ be trace class for every $\beta > 0$, and suppose that $V$ is bounded below, $\inf V = V_m$. Let $\varphi_j$ be the normalised eigenstate of $H^0$ belonging to the eigenvalue $\varepsilon_j$. Then

$$e^{-\beta\varepsilon_j}\|\varphi_j\|_\infty^2 \leqslant e^{-\beta V_m}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{d/2} \tag{22}$$

and

$$\|\varphi_j\|_\infty^2 \leqslant \left(\frac{em(\varepsilon_j - V_m)}{d\pi\hbar^2}\right)^{d/2}. \tag{23}$$

*Proof.*

$$e^{-\beta\varepsilon_j} |\varphi_j(\mathbf{r})|^2 \leqslant \sum_i e^{-\beta\varepsilon_i} |\varphi_i(\mathbf{r})|^2 = \langle\mathbf{r}| e^{-\beta H^0} |\mathbf{r}\rangle$$

$$= \int P_{00}^\beta(\mathrm{d}\omega) \, e^{-\int_0^\beta V(\mathbf{r}+\omega(s)) \, \mathrm{d}s} \leqslant e^{-\beta V_m} \lambda_\beta^{-d} \qquad (24)$$

which, after taking the supremum on the left-hand side, is (22). Multiplying by $e^{\beta\varepsilon_j}$ and minimizing the right member with respect to $\beta$ yields (23).

We note that for sufficiently fast increasing potentials $H^0$ is ultracontractive and the normalized eigenstates are uniformly bounded.[4, 5] In particular, this obviously holds true for a particle confined in a rectangular domain with Dirichlet, Neumann or periodic boundary conditions. All our results cover these cases. However, in the present paper we need only the weaker bound (22) on the eigenfunctions.

## 3. FREE BOSE GAS IN A DEEP TRAP

$N$ noninteracting bosons in a deep trap are described by the Hamiltonian

$$H_N^0 = \sum_{i=1}^N H^0(i) = T_N + \sum_{i=1}^N V(\mathbf{r}_i) \qquad T_N = -\frac{\hbar^2}{2m} \sum_{i=1}^N \Delta_i. \qquad (25)$$

We can consider $H_N^0$ directly in infinite space, because $\exp(-\beta H_N^0)$ is a trace class operator on $L^2(\mathbb{R}^{dN})$. Therefore, to perform a thermodynamic limit it remains sending $N$ to infinity.

Let $Z[\beta H_N^0]$ denote the canonical partition function for $N$ bosons. We have the following.

**Proposition 3.1.**   The limit

$$\lim_{N\to\infty} e^{\beta N\varepsilon_0} Z[\beta H_N^0] \equiv e^{-\beta F_0(\beta)} \qquad (26)$$

exists, and $F_0(\beta)$ is an analytic function of $\beta$ for any $\beta > 0$.

*Proof.*   Let $n_j \geqslant 0$ denote the number of bosons in the $j$th eigenstate of $H^0$. Then

$$Z[\beta H_N^0] = \sum_{\{n_j\}:\, \sum n_j = N} e^{-\beta \sum n_j \varepsilon_j} = \sum_{N'=0}^N e^{-\beta(N-N')\varepsilon_0} \sum_{\{n_j\}_{j>0}:\, \sum n_j = N'} e^{-\beta \sum n_j \varepsilon_j}. \qquad (27)$$

Therefore

$$e^{\beta N \varepsilon_0} Z[\beta H_N^0] = \sum_{\{n_j\}_{j>0} \,:\, \sum n_j \,\leqslant\, N} e^{-\beta \sum n_j (\varepsilon_j - \varepsilon_0)}, \tag{28}$$

so that

$$\lim_{N \to \infty} e^{\beta N \varepsilon_0} Z[\beta H_N^0] = \sum_{\{n_j\}_{j>0} \,:\, \sum n_j \,<\, \infty} e^{-\beta \sum n_j (\varepsilon_j - \varepsilon_0)}$$
$$= \prod_{j=1}^{\infty} \sum_{n_j=0}^{\infty} e^{-\beta n_j (\varepsilon_j - \varepsilon_0)} = \prod_{j=1}^{\infty} \frac{1}{1 - e^{-\beta(\varepsilon_j - \varepsilon_0)}} \tag{29}$$

and

$$\beta F_0(\beta) = \sum_{j=1}^{\infty} \ln(1 - e^{-\beta(\varepsilon_j - \varepsilon_0)}). \tag{30}$$

To conclude, we need a lemma.

**Lemma 3.2.** Let $|a_n| < 1$ and $\sum_{n=1}^{\infty} |a_n| < \infty$. Then $\sum_{n=1}^{\infty} \ln(1 - a_n)$ is absolutely convergent.

*Proof.* One can choose $N$ such that $|a_n| < 1/2$ if $n \geqslant N$. Then

$$\sum_{n=N}^{\infty} |\ln(1-a_n)| = \sum_{n=N}^{\infty} \left| \sum_{l=1}^{\infty} \frac{a_n^l}{l} \right| \leqslant \sum_{n=N}^{\infty} \sum_{l=1}^{\infty} \frac{|a_n|^l}{l}$$
$$= \sum_{n=N}^{\infty} |a_n| \sum_{l=1}^{\infty} \frac{|a_n|^{l-1}}{l} \leqslant 2 \ln 2 \sum_{n=N}^{\infty} |a_n| < \infty$$

which proves the lemma.

Because $e^{-\beta H^0}$ is trace class for any $\beta > 0$, the conditions of the lemma hold for $a_n = \exp(-z(\varepsilon_n - \varepsilon_0))$ if $z \in \mathbb{C}$, $\operatorname{Re} z > 0$. Thus, for any $\epsilon > 0$, $\sum_{n=1}^{\infty} \ln(1 - \exp(-z(\varepsilon_n - \varepsilon_0)))$ is uniformly absolute convergent in the half-plane $\operatorname{Re} z \geqslant \epsilon$. Since every term is analytic, the sum will be analytic as well. This finishes the proof of the proposition.

The peculiar feature of the infinite system is clearly shown by Eq. (26). The total free energy of the gas is

$$-\beta^{-1} \ln Z[\beta H_N^0] = N \varepsilon_0 + F_0(\beta) + o(1). \tag{31}$$

This means that there is no phase transition and the free energy per particle of the infinite system is $\varepsilon_0$ at any temperature. Thus, at any $\beta > 0$ the gas is

in a low-temperature phase which is a nonextensive perturbation of the ground state: *All but a vanishing fraction of the particles are in the condensate!* Below we make this observation quantitative.

Let $P_{\beta H_N^0}(A)$ denote the probability of an event $A$ according to the canonical Gibbs measure. Let $N' = N - n_0$, the number of particles in the excited states of $H^0$. First, notice that in the infinite system the probability that all the particles are in the ground state is positive at any temperature: From Eq. (27),

$$P_{\beta H_N^0}(N' = 0) = \frac{e^{-\beta N \varepsilon_0}}{Z[\beta H_N^0]} \to e^{\beta F_0(\beta)} \qquad \text{as} \quad N \to \infty \tag{32}$$

which tends continuously to zero only when $\beta \to 0$. More precise informations can also be obtained. For an integer $m$ between 0 and $N$, with Proposition 3.1 we find

$$P_{\beta H_N^0}(N' \geqslant m) = P_{\beta H_N^0}(N' = 0) \sum_{\{n_j\}_{j>0} \,:\, m \leqslant \sum n_j \leqslant N} e^{-\beta \sum n_j(\varepsilon_j - \varepsilon_0)}. \tag{33}$$

A lower bound is obtained by keeping a single term, $n_1 = m$, $n_j = 0$ for $j > 1$:

$$P_{\beta H_N^0}(N' \geqslant m) \geqslant P_{\beta H_N^0}(N' = 0) \, e^{-\beta m(\varepsilon_1 - \varepsilon_0)}. \tag{34}$$

If we replace $m$ by any increasing sequence $a_N$, this yields

$$\liminf_{N \to \infty} \frac{1}{a_N} \ln P_{\beta H_N^0}(N' \geqslant a_N) \geqslant -\beta(\varepsilon_1 - \varepsilon_0). \tag{35}$$

To obtain an upper bound, choose any $\mu$ with $0 \leqslant \mu < \varepsilon_1 - \varepsilon_0$. Then

$$\begin{aligned}
P_{\beta H_N^0}(N' \geqslant m) \\
&= P_{\beta H_N^0}(N' = 0) \sum_{N' = m}^{N} e^{-\beta \mu N'} \sum_{\{n_j\}_{j>0} \,:\, \sum n_j = N'} e^{-\beta \sum n_j(\varepsilon_j - \varepsilon_0 - \mu)} \\
&\leqslant P_{\beta H_N^0}(N' = 0) \, e^{-\beta \mu m} \prod_{j=1}^{\infty} \frac{1}{1 - e^{-\beta(\varepsilon_j - \varepsilon_0 - \mu)}} \\
&= P_{\beta H_N^0}(N' = 0) \, Q(\beta, \mu) \, e^{-\beta \mu m}
\end{aligned} \tag{36}$$

where $Q(\beta, \mu)$ is defined by the last equality. Notice that $Q(\beta, 0) = e^{-\beta F_0(\beta)}$. The inequality has been obtained by first bounding $e^{-\beta \mu N'}$ above by $e^{-\beta \mu m}$

and then by extending the summation over $N'$ from 0 to infinity. Again, for $m = a_N \to \infty$,

$$\limsup_{N \to \infty} \frac{1}{a_N} \ln P_{\beta H_N^0}(N' \geq a_N) \leq -\beta\mu. \tag{37}$$

This being true for all $\mu < \varepsilon_1 - \varepsilon_0$, it holds also for $\mu = \varepsilon_1 - \varepsilon_0$, so the lower bound found in (35) is an upper bound as well, and (35) and (37) together yield

**Proposition 3.3.** If $0 < a_N \leq N$ and $a_N$ tends to infinity, then

$$\lim_{N \to \infty} \frac{1}{a_N} \ln P_{\beta H_N^0}(N' \geq a_N) = -\beta(\varepsilon_1 - \varepsilon_0). \tag{38}$$

By the Borel–Cantelli lemma, inequality (36) implies that $N'$ is finite with probability 1 when $N$ is infinite. Moreover, its expectation value is also finite: for any $\mu \in (0, \varepsilon_1 - \varepsilon_0)$ we have

$$\langle N' \rangle_{\beta H_N^0} \leq \frac{P_{\beta H_N^0}(N' = 0)\, Q(\beta, \mu)}{(1 - e^{-\beta\mu})^2} \tag{39}$$

so that

$$\lim_{N \to \infty} \langle N' \rangle_{\beta H_N^0} \leq \inf_{0 < \mu < \varepsilon_1 - \varepsilon_0} \frac{Q(\beta, \mu)}{Q(\beta, 0)} \frac{1}{(1 - e^{-\beta\mu})^2}. \tag{40}$$

More generally, all moments of $N'$ remain finite as $N \to \infty$:

$$\lim_{N \to \infty} \langle (N')^k \rangle_{\beta H_N^0} \leq \inf_{0 < \mu < \varepsilon_1 - \varepsilon_0} \frac{Q(\beta, \mu)}{Q(\beta, 0)} \frac{d^k}{d(-\beta\mu)^k} \frac{1}{1 - e^{-\beta\mu}}. \tag{41}$$

This fact will be used in the proof of Theorem 2.

Let us summarize the results of this section:

**Theorem 3.4.** $N$ noninteracting bosons in a deep trap with eigen-energies $\varepsilon_0 < \varepsilon_1 \leq \cdots$ have a free energy $N\varepsilon_0 + F_0(\beta) + o(1)$, where $F_0$ is an analytic function of $\beta$ for any $\beta > 0$. There is no phase transition in any dimension, however, for any $d \geq 1$, the infinite system is in a low-temperature phase ($T_c = \infty$): At any finite temperature, all but a finite expected number of bosons are in the one-particle ground state.

The conclusions about Bose–Einstein condensation are not modified if the ground state of $H^0$ is degenerate. If

$$\varepsilon_0 = \cdots = \varepsilon_J < \varepsilon_{J+1} \leqslant \cdots, \tag{42}$$

we define $N' = N - (n_0 + \cdots + n_J)$. Then, the earlier formulas remain valid if in the summations and products $j > 0$ is replaced by $j > J$, and $\varepsilon_1 - \varepsilon_0$ is replaced by $\varepsilon_{J+1} - \varepsilon_0$. In particular, all moments of $N'$ are bounded and we have a 100% condensation into the finite dimensional subspace of ground states. This remark is relevant, e.g., for bosons with an internal degree of freedom (spin).

## 4. CONDENSATION OF INTERACTING BOSONS

### 4.1. The Order We Are Looking for

Due to the pioneering work of Penrose[6] and subsequent papers by Penrose and Onsager[7] and Yang,[8] it is generally understood and agreed that Bose–Einstein condensation, from a mathematical point of view, is an intrinsic property of the one-particle reduced density matrix, $\sigma_1$, and means that the largest eigenvalue of $\sigma_1$, which is equal to its norm, $\|\sigma_1\|$, is of the order of $N$. For the homogeneous gas the equivalence of this physically not very appealing definition with the existence of an off-diagonal long-range order, showing up in the coordinate space representation (integral kernel) of $\sigma_1$, was demonstrated in ref. 7. For a trapped gas it is intuitively more satisfactory to define BEC as the accumulation of a macroscopic number of particles in a single-particle state. The proof that this is meaningful, whether or not there is interaction, and equivalent with $\|\sigma_1\| = O(N)$, is the subject of this section.

Following the general setting of ref. 8, let $\sigma$ be a density matrix, i.e., a positive operator of trace 1 acting in $\mathscr{H}^N$, where $\mathscr{H}$ is a one-particle separable Hilbert space. Permutations of the $N$ particles can be defined as unitary operators in $\mathscr{H}^N$, and $\sigma$ is supposed to commute with all of them. The associated one-particle reduced density matrix, $\sigma_1$, is a positive operator of trace $N$ in $\mathscr{H}$, obtained by taking the sum of the partial traces of $\sigma$ over the $N-1$-particle subspaces: If $\{\varphi_n\}_{n=0}^{\infty}$ is any orthonormal basis in $\mathscr{H}$ and $\phi$ and $\psi$ are any elements of $\mathscr{H}$ then

$$(\phi, \sigma_1 \psi) \equiv \sum_{j=1}^{N} \sum_{\{i_k\}_{k \neq j}} (\varphi_{i_1} \cdots \varphi_{i_{j-1}} \phi \varphi_{i_{j+1}} \cdots \varphi_{i_N}, \sigma \, \varphi_{i_1} \cdots \varphi_{i_{j-1}} \psi \varphi_{i_{j+1}} \cdots \varphi_{i_N})$$

$$= N \sum_{i_2, \ldots, i_N} (\phi \varphi_{i_2} \cdots \varphi_{i_N}, \sigma \, \psi \varphi_{i_2} \cdots \varphi_{i_N}) \tag{43}$$

because of the permutation-invariance of $\sigma$. In (43) the summation over each $i_k$ is unrestricted and the matrix elements of $\sigma$ are taken with simple (non-symmetrized) tensor products ($\otimes$ omitted).

Let $\varphi_0$ be any normalized element of $\mathscr{H}$. We define the *mean* (with respect to $\sigma$) *number of particles occupying* $\varphi_0$ as follows. We complete $\varphi_0$ into an orthonormal basis $\{\varphi_n\}_{n=0}^{\infty}$ of $\mathscr{H}$. In $\mathscr{H}^N$ we use the product basis

$$\{\Phi_{\mathbf{i}} = \varphi_{i_1} \otimes \cdots \otimes \varphi_{i_N} \mid \mathbf{i} = (i_1, \cdots, i_N) \in \mathbb{N}^N\}. \qquad (44)$$

To $\varphi_0$ and $\Phi_{\mathbf{i}}$ we assign

$$n[\varphi_0](\mathbf{i}) \equiv \sum_{j=1}^{N} |(\varphi_0, \varphi_{i_j})|^2 = \sum_j \delta_{i_j, 0}, \qquad (45)$$

which is the number of particles in the state $\varphi_0$ among $N$ particles occupying the states $\varphi_{i_1}$,..., $\varphi_{i_N}$, respectively. We can use (45) to define $n[\varphi_0]$ as a positive operator in $\mathscr{H}^N$. Alternately, we can interprete $(\Phi_{\mathbf{i}}, \sigma\Phi_{\mathbf{i}})$ as the probability of $\Phi_{\mathbf{i}}$ and $n[\varphi_0]$ as a random variable over this probability field. In any case, the mean value of $n[\varphi_0]$ with respect to $\sigma$ is

$$\begin{aligned}
\langle n[\varphi_0] \rangle_\sigma &\equiv \operatorname{Tr} n[\varphi_0]\, \sigma = \sum_{i_1,...,i_N} \sum_{j=1}^{N} \delta_{i_j, 0} (\Phi_{\mathbf{i}}, \sigma\Phi_{\mathbf{i}}) \\
&= \sum_{j=1}^{N} \sum_{i_j} \delta_{i_j, 0} \sum_{\{i_k\}_{k \neq j}} (\Phi_{\mathbf{i}}, \sigma\Phi_{\mathbf{i}}) = \frac{1}{N} \sum_{j=1}^{N} \sum_{i_j} \delta_{i_j, 0} (\varphi_{i_j}, \sigma_1 \varphi_{i_j}) \\
&= \sum_{i=0}^{\infty} \delta_{i, 0} (\varphi_i, \sigma_1 \varphi_i) = (\varphi_0, \sigma_1 \varphi_0), \qquad (46)
\end{aligned}$$

an intrinsic quantity independent of the basis. Reading Eq. (46) in the opposite sense, we find that, whether or not there is interaction, *the physical meaning of* $(\varphi_0, \sigma_1\varphi_0)$ *is the average number of particles in the single particle state* $\varphi_0$. Since $\|\sigma_1\| = \sup_{\|\varphi\|=1}(\varphi, \sigma_1\varphi)$, we obtained the following result.

**Proposition 4.1.** There is BEC in the sense that $\lim_{N \to \infty} \|\sigma_1\|/N > 0$ if and only if there exists a macroscopically occupied $\varphi_0 \in \mathscr{H}$ (which may depend on $N$), i.e., $\lim_{N \to \infty} \langle n[\varphi_0] \rangle_\sigma/N > 0$.

The proposition is valid with obvious modifications also in the homogeneous case. The choice of the macroscopically occupied single particle state is not unique. Highest occupation is obtained for the dominant eigenvector, $\psi_{\sigma_1}$, of $\sigma_1$ (the one belonging to the largest eigenvalue), in which case $\langle n[\psi_{\sigma_1}] \rangle_\sigma = \|\sigma_1\|$. Any other state having a nonvanishing

overlap in the limit $N \to \infty$ with $\psi_{\sigma_1}$ can serve for proving BEC. We can even find an infinite orthogonal family of vectors, all having a nonvanishing asymptotic overlap with $\psi_{\sigma_1}$. One can speak about a generalized condensation [9] only when the occupation of more than one eigenstate of $\sigma_1$ becomes asymptotically divergent. In the noninteracting gas $\psi_{\sigma_1}$ is just the ground state of the one-body Hamiltonian.

The homogeneous gas represents a particular case. Namely, $\psi_{\sigma_1}(\mathbf{r}) = \psi_{\mathbf{k}=0}^L(\mathbf{r}) \equiv 1/L^{d/2}$ for any translation invariant interaction, if the gas is confined in a cube of side $L$ and the boundary condition is periodic. Indeed, in this case $\sigma_1$ is diagonal in momentum representation, therefore $\psi_{\mathbf{k}}^L(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/L^{d/2}$ are its eigenstates. On the other hand, the integral kernel $\langle \mathbf{r}| \sigma_1 |\mathbf{r}'\rangle$ is positive (now we speak about $\sigma \sim \exp(-\beta H)$ in the bosonic subspace or $\sigma = |\Psi\rangle\langle\Psi|$ where $\Psi(\mathbf{r}_1,...,\mathbf{r}_N)$ is a translation invariant positive symmetric function), and by a suitable generalization of the Perron–Frobenius theorem (see, e.g., ref. 10) the constant vector must be the dominant eigenvector. This is presumably the only case when the ground state of the one-body Hamiltonian remains the dominant eigenvector of the one-particle reduced density matrix for the interacting system, yet there exists no proof of a macroscopic occupation of this state in the presence of interactions (unless a gap is introduced in the excitation spectrum[11]).

In the case of a trapped gas we do not generally know the dominant eigenvector of $\sigma_1$. However, we can carry through the proof by the use of the low energy eigenstates of $H^0$.

## 4.2. Interacting Bosons in a Deep Trap

In this section we ask about condensation of interacting bosons in a deep trap. Let $U_N: \mathbb{R}^{dN} \to \mathbb{R}$ be a symmetric function of $\mathbf{r}_1,...,\mathbf{r}_N$ which is bounded below, and define

$$H_N = H_N^0 + U_N. \tag{47}$$

We can consider $H_N$ directly in infinite space, because $\exp(-\beta H_N)$ is a trace class operator on $L^2(\mathbb{R}^{dN})$. So as in Section 3, the thermodynamic limit means $N$ tending to infinity. The canonical partition function will be denoted by $Z[\beta H_N]$. The density matrix is

$$\sigma = P_N^+ e^{-\beta H_N}/Z[\beta H_N] \tag{48}$$

where $P_N^+ = (1/N!) \sum_{\pi \in S_N} \pi$ is the orthogonal projection to the symmetric subspace of $\mathscr{H}^N$ and $Z[\beta H_N] = \mathrm{Tr}\, P_N^+ e^{-\beta H_N}$.

We want to prove the persistence of BEC in the presence of interaction, that is, the continuity of the low-temperature phase as $U_N$ increases from zero to a finite strength. This will be achieved by proving macroscopic occupation of at least one low-lying eigenstate of $H^0$, which may depend on the interaction strength. We cannot expect, and will not obtain, a 100% condensation because the overlap of any eigenstate of $H^0$ with $\psi_{\sigma_1}$ must be smaller than 1. (The 100% condensation[1] into $\phi_{GP}$, the minimizer of the Gross–Pitaevskii functional, found for the ground state of interacting gases in the dilute limit in locally bounded traps, means that $(\phi_{GP}, \psi_{\sigma_1}) \to 1$ as $N \to \infty$. In this case $\sigma = |\Psi\rangle\langle\Psi|$, where $\Psi$ is the unknown ground state.)

In the proof of the next theorem we use the basis of the $H^0$ eigenstates, given by $H^0\varphi_j = \varepsilon_j\varphi_j$, and the symmetric and normalized eigenstates of $H_N^0$: $|\mathbf{n}\rangle = |n_0, n_1, \ldots\rangle$ is the symmetrized product state of norm 1 containing $n_j$ times the factor $\varphi_j$, where $\sum n_j = N$. For the sake of clarity, we restrict the discussion to the case when the ground state of $H^0$ is nondegenerate, and use the notation $\Phi_0$ for the (unique) ground state of $H_N^0$, given by $n_0 = N$ and $n_j = 0$, $j > 0$. Extension to the case of spin- or spatial degeneracy is straightforward.

**Theorem 4.2.**   Let

$$L(U) \equiv \limsup_{N \to \infty} \frac{1}{N}\left[(\Phi_0, U_N\Phi_0) - \inf U_N\right]. \tag{49}$$

For any $d \geqslant 1$ the following hold true.

(i)   If $L(U) < \infty$, at zero temperature there is Bose–Einstein condensation. Namely, if $J \geqslant 0$ is the unique integer defined by the inequalities

$$\varepsilon_J - \varepsilon_0 \leqslant L(U) < \varepsilon_{J+1} - \varepsilon_0, \tag{50}$$

for $\beta = \infty$ we have

$$\liminf_{N \to \infty} \frac{1}{N} \sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N} \geqslant 1 - \frac{L(U)}{\varepsilon_{J+1} - \varepsilon_0}. \tag{51}$$

(ii)   If $U_N$ is a stable integrable pair interaction,

$$U_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{1 \leqslant i < j \leqslant N} u_N(\mathbf{r}_i - \mathbf{r}_j), \tag{52}$$

with $\|u_N\|_1 = O(1/N)$, then $L(U) < \infty$ and for any $\beta > 0$ there is Bose–Einstein condensation and (51) holds true.

We note that in part (i) $U_N$ can be any self-adjoint operator in $L^2(\mathbb{R}^d)^{\otimes N}$ which is bounded below and leaves the symmetric subspace invariant.

*Proof.* In the first part of the proof we apply convexity inequalities in a similar manner as they were used in ref. 11.

We define a one-parameter family of one-particle Hamiltonians

$$H^0(\delta) = \sum_{j=0}^{J} (\varepsilon_j + \delta) P_j + \sum_{j=J+1}^{\infty} \varepsilon_j P_j \tag{53}$$

where $\delta$ is a real parameter and $P_j$ is the orthogonal projection onto $\varphi_j$. Let $H_N^0(\delta)$ be the corresponding Hamiltonian of $N$ noninteracting particles and $H_N(\delta) = H_N^0(\delta) + U_N$. For $\delta = 0$ we shall keep the original notation. Because

$$\sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N^{(0)}(\delta)} = -\frac{\partial \ln Z[\beta H_N^{(0)}(\delta)]}{\partial(\beta\delta)} \tag{54}$$

and the second derivative is the variance of $\sum_{j=0}^{J} n_j$, $\ln Z[\beta H_N^{(0)}(\delta)]$ are convex (decreasing) functions of $\beta\delta$. Therefore, for any $\delta > 0$

$$\sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N} \geq \frac{1}{\beta\delta} \ln \frac{Z[\beta H_N]}{Z[\beta H_N(\delta)]}$$
$$\sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N^0(\delta)} \leq \frac{1}{\beta\delta} \ln \frac{Z[\beta H_N^0]}{Z[\beta H_N^0(\delta)]} \tag{55}$$

Combining (55) with a double application of the Bogoliubov convexity inequality,[12]

$$\ln \frac{Z[\beta H_N]}{Z[\beta H_N^0]} \geq -\beta\langle U_N \rangle_{\beta H_N^0} \qquad \ln \frac{Z[\beta H_N^0(\delta)]}{Z[\beta H_N(\delta)]} \geq \beta\langle U_N \rangle_{\beta H_N(\delta)}, \tag{56}$$

we find

$$\sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N} \geq \sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N^0(\delta)} - \frac{1}{\delta} \left[ \langle U_N \rangle_{\beta H_N^0} - \langle U_N \rangle_{\beta H_N(\delta)} \right]$$
$$\geq \langle n_0 \rangle_{\beta H_N^0(\delta)} - \frac{1}{\delta} \left[ \langle U_N \rangle_{\beta H_N^0} - \inf U_N \right]. \tag{57}$$

For $\delta < \varepsilon_{J+1} - \varepsilon_0$, $\varphi_0$ is the unique ground state of $H^0(\delta)$, and thus the results of Section 3 remain valid to $H_N^0(\delta)$. At zero temperature the inequality (57) reads

$$\lim_{\beta \to \infty} \sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N} \geqslant N - \frac{1}{\delta} \left[ (\Phi_0, U_N \Phi_0) - \inf U_N \right]. \tag{58}$$

Dividing by $N$, taking the liminf as $N$ tends to infinity and then letting $\delta$ tend to $\varepsilon_{J+1} - \varepsilon_0$, we obtain part (i) of the theorem.

Suppose now that the conditions of part (ii) hold true. Stability means $\inf U_N \geqslant -BN$ for some constant $B$. On the other hand,

$$\begin{aligned}
|(\Phi_0, U_N \Phi_0)| &= \binom{N}{2} \left| \int \varphi_0(\mathbf{x})^2 \, u_N(\mathbf{x} - \mathbf{y}) \, \varphi_0(\mathbf{y})^2 \, d\mathbf{x} \, d\mathbf{y} \right| \\
&= \binom{N}{2} (2\pi)^{d/2} \left| \int \hat{u}_N(\mathbf{q}) \, |\widehat{\varphi_0^2}(\mathbf{q})|^2 \, d\mathbf{q} \right| \\
&\leqslant \binom{N}{2} \|u_N\|_1 \, \|\varphi_0^4\|_1 = O(N),
\end{aligned} \tag{59}$$

therefore

$$L(U) \leqslant \tfrac{1}{2} \|\varphi_0^4\|_1 \, \lim \sup(N \, \|u_N\|_1) + B < \infty. \tag{60}$$

Fix $J$ according to (50). Dividing (57) by $N$, taking the liminf as $N$ tends to infinity and then letting $\delta$ tend to $\varepsilon_{J+1} - \varepsilon_0$, we arrive at

$$\liminf_{N \to \infty} \frac{1}{N} \sum_{j=0}^{J} \langle n_j \rangle_{\beta H_N} \geqslant 1 - \frac{1}{\varepsilon_{J+1} - \varepsilon_0} \lim_{N \to \infty} \sup \frac{1}{N} \left[ \langle U_N \rangle_{\beta H_N^0} - \inf U_N \right]. \tag{61}$$

Here we used (40) to obtain $\langle n_0 \rangle_{\beta H_N^0(\delta)} / N = 1 - \langle N' \rangle_{\beta H_N^0(\delta)} / N \to 1$ as $N$ tends to infinity. Next we prove that for any $\beta > 0$

$$\lim_{N \to \infty} \frac{1}{N} \left[ (\Phi_0, U_N \Phi_0) - \langle U_N \rangle_{\beta H_N^0} \right] = 0. \tag{62}$$

Equations (61) and (62) clearly imply (ii).

Let $a(\mathbf{x})$ and $a(\mathbf{x})^*$ be the boson field operators, then $U_N$ is the restriction of

$$U = \tfrac{1}{2} \int a(\mathbf{x})^* \, a(\mathbf{y})^* \, u_N(\mathbf{x} - \mathbf{y}) \, a(\mathbf{x}) \, a(\mathbf{y}) \, d\mathbf{x} \, d\mathbf{y} \tag{63}$$

to the $N$-particle subspace. Denote $a_i$ and $a_i^*$ the annihilation and creation operators of a particle in the state $\varphi_i$, respectively. We have

$$a_i = \int \varphi_i(\mathbf{x})\, a(\mathbf{x})\, \mathrm{d}\mathbf{x}, \qquad a(\mathbf{x}) = \sum_{i=0}^{\infty} a_i \overline{\varphi_i}(\mathbf{x}) \tag{64}$$

and

$$U = \sum_{i,j,k,l=0}^{\infty} u_{ijkl}\, a_i^* a_j^* a_k a_l \tag{65}$$

with

$$u_{ijkl} = \int \varphi_i(\mathbf{x})\, \varphi_j(\mathbf{y})\, u_N(\mathbf{x}-\mathbf{y})\, \overline{\varphi_k}(\mathbf{x})\, \overline{\varphi_l}(\mathbf{y})\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{y}. \tag{66}$$

Now

$$\langle \mathbf{n}|\, U\, |\mathbf{n}\rangle = \sum_i u_{iiii} \binom{n_i}{2} + \sum_{i<j} (u_{ijij} + u_{ijji})\, n_i n_j \tag{67}$$

and thus

$$\begin{aligned}
\langle U_N \rangle_{\beta H_N^0} &= \frac{1}{2} \sum_i u_{iiii} \langle n_i(n_i-1)\rangle_{\beta H_N^0} + \sum_{i<j} (u_{ijij} + u_{ijji}) \langle n_i n_j \rangle_{\beta H_N^0} \\
&= \frac{1}{2} u_{0000} \langle n_0(n_0-1)\rangle_{\beta H_N^0} + R_N \\
&= (\Phi_0, U_N \Phi_0) \left\langle \left(1 - \frac{N'}{N}\right)\left(1 - \frac{N'}{N-1}\right) \right\rangle_{\beta H_N^0} + R_N
\end{aligned} \tag{68}$$

where

$$R_N = \tfrac{1}{2} \sum_{i>0} u_{iiii} \langle n_i(n_i-1)\rangle_{\beta H_N^0} + \sum_{0 \leqslant i < j} (u_{ijij} + u_{ijji}) \langle n_i n_j \rangle_{\beta H_N^0}. \tag{69}$$

First we estimate the residue $R_N$. Because

$$\max\{|u_{ijij}|, |u_{ijji}|\} \leqslant \|\varphi_i\|_\infty\, \|\varphi_j\|_\infty\, \|u_N\|_1, \tag{70}$$

$$|R_N| \leqslant \|u_N\|_1 \left( \tfrac{1}{2} \sum_{i>0} \|\varphi_i\|_\infty^2 \langle n_i(n_i-1)\rangle_{\beta H_N^0} + 2 \sum_{0 \leqslant i < j} \|\varphi_i\|_\infty\, \|\varphi_j\|_\infty\, \langle n_i n_j \rangle_{\beta H_N^0} \right). \tag{71}$$

There is some constant $c_1(\beta)$ such that for any $i, j > 0$

$$\langle n_i(n_i - 1)\rangle_{\beta H_N^0} \leqslant c_1(\beta) \, e^{-2\beta(\varepsilon_i - \varepsilon_0)}$$
$$\langle n_i n_j\rangle_{\beta H_N^0} \leqslant c_1(\beta) \, e^{-\beta(\varepsilon_i - \varepsilon_0)}e^{-\beta(\varepsilon_j - \varepsilon_0)}. \tag{72}$$

These inequalities can be shown by direct estimation. Also, both expectation values can asymptotically be computed by using the asymptotic ($N \to \infty$) factorization of the probability measure,

$$P_{\beta H_N^0}(\{n_j\}_{j > 0}) \asymp \prod_{j=1}^{\infty} (1 - e^{-\beta(\varepsilon_j - \varepsilon_0)}) \, e^{-\beta(\varepsilon_j - \varepsilon_0) \, n_j}. \tag{73}$$

With another suitable constant $c_2(\beta)$ we obtain

$$\frac{1}{2} \sum_{i > 0} \|\varphi_i\|_\infty^2 \, \langle n_i(n_i - 1)\rangle_{\beta H_N^0} + 2 \sum_{0 < i < j} \|\varphi_i\|_\infty \, \|\varphi_j\|_\infty \, \langle n_i n_j\rangle_{\beta H_N^0}$$

$$\leqslant c_2(\beta) \left( \sum_{i=1}^{\infty} \|\varphi_i\|_\infty \, e^{-\beta(\varepsilon_i - \varepsilon_0)} \right)^2$$

$$\leqslant c_2(\beta) \, e^{\beta(\varepsilon_0 - V_m)} \left( \frac{m}{2\pi\hbar^2\beta} \right)^{d/2} (\mathrm{tr} \, e^{-\frac{\beta}{2}(H^0 - \varepsilon_0)} - 1)^2 \equiv \tilde{c}(\beta). \tag{74}$$

In the last inequality we used the bound

$$\|\varphi_i\|_\infty \, e^{-\frac{\beta}{2}(\varepsilon_i - \varepsilon_0)} \leqslant e^{\frac{\beta}{2}(\varepsilon_0 - V_m)} \left( \frac{m}{2\pi\hbar^2\beta} \right)^{d/4} \tag{75}$$

obtained in Proposition 2.2. The remaining term

$$2 \|\varphi_0\|_\infty \sum_{j=1}^{\infty} \|\varphi_j\|_\infty \, \langle n_0 n_j\rangle_{\beta H_N^0} \leqslant 2N \|\varphi_0\|_\infty \sum_{j=1}^{\infty} \|\varphi_j\|_\infty \, \langle n_j\rangle_{\beta H_N^0} \leqslant c(\beta) \, N \tag{76}$$

because for $j > 0$, $\langle n_j\rangle_{\beta H_N^0} \sim e^{-\beta(\varepsilon_j - \varepsilon_0)}$. Hence,

$$\frac{1}{N} |R_N| \leqslant \|u_N\|_1 \left( c(\beta) + \frac{\tilde{c}(\beta)}{N} \right) \to 0 \qquad \text{as} \quad N \to \infty. \tag{77}$$

Therefore,

$$\lim_{N \to \infty} \frac{1}{N} [(\Phi_0, U_N \Phi_0) - \langle U_N\rangle_{\beta H_N^0}]$$

$$= \lim_{N \to \infty} \frac{1}{N} (\Phi_0, U_N \Phi_0) \left[ 1 - \left\langle \left( 1 - \frac{N'}{N} \right)\left( 1 - \frac{N'}{N - 1} \right) \right\rangle_{\beta H_N^0} \right] = 0 \tag{78}$$

because the difference in the square bracket is of order $1/N$, cf. (41), and its prefactor is of order 1, see (59). This finishes the proof of the theorem.

Notice that in the proof of (77) and (78) we have used only $\|u_N\|_1 = o(1)$. The condition of integrability of $u_N$ could be relaxed. For example, if $u$ is a bounded function (or $u$ is integrable and bounded below), the theorem holds for $u_N = (1/N)\, u$, which is a mean-field interaction. More interesting examples are provided by scaled interactions.

**Corollary 4.3.** Let $u: \mathbb{R}^d \to \mathbb{R}$ be an integrable nonnegative function. Suppose we are given two positive sequences $\alpha_N$ and $b_N$ satisfying the condition

$$S \equiv \sup_N \, b_N \alpha_N^{-d} N < \infty. \tag{79}$$

Then for any $\beta > 0$ there is Bose–Einstein condensation for the interaction

$$u_N(\mathbf{x}) = b_N u(\alpha_N \mathbf{x}). \tag{80}$$

*Proof.* $U_N$ is an integrable stable pair interaction ($\inf U_N = 0$) and

$$\|u_N\|_1 = b_N \alpha_N^{-d} \, \|u\|_1 \leqslant \frac{S \, \|u\|_1}{N}. \tag{81}$$

Thus, the conditions of part (ii) of the theorem are verified.

### Remarks.

**1.** If $\alpha_N$ is constant, we obtain the mean-field interaction. If $\alpha_N$ is strictly monotonous, it can be inverted and, hence, $b_N$ may depend on $N$ only via $\alpha_N$. For example, $\alpha_N = N^\eta$ and $b_N = \alpha_N^{d-1/\eta}$ satisfy (79).

**2.** If the scattering length of $u$ is $a$ and $b_N = \alpha_N^2$ then the scattering length of $u_N$ is $a/\alpha_N$. To see this, we recall (cf. ref. 13) the definition of the scattering length:

Let $V$ be a spherical finite-range potential such that $-\frac{\hbar^2}{2m}\Delta + V$ has no negative or zero energy bound state. Then the Schrödinger equation written for zero energy,

$$-\frac{\hbar^2}{2m}\Delta\phi(\mathbf{x}) + V(\mathbf{x})\,\phi(\mathbf{x}) = 0 \tag{82}$$

has a (up to constant multipliers) unique spherical sign-keeping solution, $\phi_0$. If $r = |\mathbf{x}| > R_0$, the range of the potential, this solution reads

$$\phi_0(\mathbf{x}) = \begin{cases} 1 - (a/r)^{d-2} & \text{if} \quad d \neq 2 \\ \ln(r/a) & \text{if} \quad d = 2 \end{cases} \tag{83}$$

with some $a \leqslant R_0$. We call $a$ the scattering length of $V$ and $\phi_0$ the defining solution. To obtain the scattering length of a pair interaction $u$ one has to solve (82) with $V = u/2$, the $1/2$ accounting for the reduced mass. For a nonnegative integrable infinite range potential (pair interaction) a finite scattering length still can be defined by truncating the potential at a finite $R_0$ and taking the (finite) limit of $a(R_0)$ as $R_0 \to \infty$, see Appendix A of ref. 13.

Suppose now that the scattering length of $u$ is $a$. What is the scattering length of $u_N$, given by (80)? This is not always easy to tell because the defining solution for $u_N$ is generally in no simple relation with that one for $u$. However, from Eqs. (82) and (83) it is easily seen that the defining solutions of $u$ and

$$u_\alpha(\mathbf{x}) = \alpha^2 u(\alpha \mathbf{x}) \tag{84}$$

are related by scaling, $\phi_0[u_\alpha](\mathbf{x}) = \phi_0[u](\alpha \mathbf{x})$, and therefore the scattering length of $u_\alpha$ is $a/\alpha$.

**3.** If $\alpha_N$ tends to infinity, the scattering length of $u_N$ tends to zero, and the operator $-\frac{\hbar^2}{2m} \Delta + u_N/2$ converges in norm resolvent sense to the one-particle kinetic energy operator. For this to happen, in two and three dimensions $u_N \geqslant 0$ is essential. Indeed, in two and three dimensions with $\alpha_N$ diverging and $b_N$ chosen so that (79) is respected one could define point interactions, that is, self-adjoint extensions of the symmetric operator $-\frac{\hbar^2}{2m} \Delta|_{C_0^\infty(\mathbb{R}^d - \{0\})}$ with a nonvanishing scattering length.[14] However, it turns out that for $u_N \geqslant 0$ the only extension is the kinetic energy operator (cf. Theorems 1.2.5 and 5.5 of ref. 14). The result of Theorem 2 and its corollary can be nontrivial because the scattering length vanishes in conjunction with a diverging particle number.

**4.** In three dimensions the Gross–Pitaevskii scaling limit is obtained by fixing $Na_N$, where $a_N$ is the scattering length of the pair interaction, while $N \to \infty$. To show BEC, we choose $b_N = \alpha_N^2$ and $\alpha_N \propto N$, so that $u_N = u_{\alpha_N}$ with scattering length $a_N = a_1/N$. Observe that $\|u_{\alpha_N}\|_1 = N^{-1} \|u\|_1$ for GP scaling in three dimensions.

**5.** Let $H_N[V, u]$ be an $N$-particle Hamiltonian with an external potential $V$ and pair interaction $u$. Then

$$\beta H_N[V, \alpha_N^2 u(\alpha_N \cdot)] \cong \beta \alpha_N^2 H_N[\alpha_N^{-2} V(\alpha_N^{-1} \cdot), u]. \tag{85}$$

If $\alpha_N$ tends to infinity, the scaled temperature $(\beta\alpha_N^2)^{-1}$ goes to zero and the trap opens. Lieb and Seiringer[1] obtained results on the limit of the sequence of ground states of (85). Theorem 2 refers to the limit of the thermal equilibrium states generated by (85). It is not obvious that the two limits define the same state for $N = \infty$. In Theorem 2 there is a first hint that this may hold true: By proving Eq. (62), we obtain the same lower bound (51) on the density of the condensate at positive temperatures as at zero temperature.

**6.** In two dimensions the scattering length of $u_N$ is always smaller than $a/\alpha_N$, the scattering length of $u_{\alpha_N}$, cf. (84). In general,

$$u_N(\mathbf{x}) = b_N \alpha_N^{-2} u_{\alpha_N}(\mathbf{x}) \leqslant SN^{-1}\alpha_N^{d-2} u_{\alpha_N}(\mathbf{x}). \tag{86}$$

In particular, in two dimensions $u_N \leqslant (S/N)\, u_{\alpha_N}$. Because for $u \geqslant 0$ the scattering length of $\lambda u$ increases with $\lambda > 0$, the scattering length of any admissible $u_N$ is smaller than that of $u_{\alpha_N}$. We note that in two dimensions $\|u_\alpha\|_1 = \|u\|_1$, independently of $\alpha$.

**7.** The sequence $\alpha_N$ may also decrease with $N$, provided that $b_N$ decreases sufficiently rapidly, see, e.g., Remark 1 for $\eta < 0$. A curious example in one dimension is $\alpha_N = N^{-1}$ and $b_N = N^{-2}$. Thus, the scattering length increases proportional to $N$, instead of going to zero. According to Eq. (85), this case corresponds to closing the trap and sending the temperature to infinity—just the opposite of the Gross–Pitaevskii limit in three dimensions.

**8.** Theorem 2 is valid for a gas confined in a box with periodic, Neumann or Dirichlet boundary conditions. The geometric confinement on a $d$-torus is interesting because the eigenstates of the one-particle Hamiltonian are eigenstates of the one-particle reduced density matrix as well, see Section 4.1. Now the inequality (51) implies that at least $\varphi_0$ is macroscopically occupied and suggests that $\langle n_j \rangle$ for some small positive $j$ can also be of order $N$. This would mean a kind of generalized Bose–Einstein condensation, in contrast to the 100% condensation into a single state, obtained for locally bounded trap potentials.[1]

**9.** For bosons in a locally bounded potential trap scaling of a nonnegative interaction is unavoidable in order that condensation takes place into a fixed localized state $\varphi$. Particles in $\varphi$ are confined in a bounded box with a probability arbitrarily close to 1. An unscaled nonnegative interaction would push the particles outside this box and, hence, out of $\varphi$. In effect, with increasing $N$ the system could diminish its interaction energy at the expense of the potential energy, by letting the particles "climb" a little bit higher up in the potential well.

## ACKNOWLEDGMENTS

## REFERENCES

1. E. H. Lieb and R. Seiringer, *Phys. Rev. Lett.* **88**:170409 (2002).
2. J. Ginibre, in *Statistical Mechanics and Quantum Field Theory*, C. De Witt and R. Stora, eds. (Gordon & Breach, New York, 1971), p. 327.
3. E. C. Titchmarsh, *Eigenfunction Expansions* (Clarendon Press, Oxford, 1962), Chap. VII.
4. E. B. Davies and B. Simon, *J. Funct. Anal.* **59**:335 (1984).
5. R. Bañuelos, *J. Funct. Anal.* **100**:181 (1991).
6. O. Penrose, *Phil. Mag.* **42**:1373 (1951).
7. O. Penrose and L. Onsager, *Phys. Rev.* **104**:576 (1956).
8. C. N. Yang, *Rev. Mod. Phys.* **34**:694 (1962).
9. M. van den Berg, J. T. Lewis, and J. V. Pulè, *Helv. Phys. Acta* **59**:1271 (1986).
10. M. G. Krein and M. A. Rutman, *Am. Math. Soc. Transl. Series 1* **10**:199 (1962). [*Usp. Mat. Nauk.* **3**:3 (1948)].
11. J. Lauwers, A. Verbeure, and V. A. Zagrebnov, *J. Phys. A: Math. Gen.* **36**:L169 (2003).
12. V. A. Zagrebnov and J.-B. Bru, *Phys. Rep.* **350**:291 (2001).
13. E. H. Lieb and J. Yngvason, *J. Stat. Phys.* **103**:509 (2001).
14. S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden, *Solvable Models in Quantum Mechanics* (Springer-Verlag, New York, 1988).