Thermodynamic limit and proof of condensation for trapped bosons

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Abstract

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 the one-particle ground state persists at all temperatures.

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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 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 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 BEC at zero temperature.

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 β. 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. We want to describe BEC in analogy with phase transitions in homogeneous systems. Therefore, we study the system 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 β. There is no phase transition in any dimension $d \geq 1$, 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 less than N times the spectral gap, there is condensation into the one-particle ground state. This holds true in any dimension and at any temperature. The occupation of the one-particle ground state 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. Our examples include the Gross-Pitaevskii scaling limit.

2 One-body Hamiltonian for deep traps

The one-particle Hamiltonian we are going to use is

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

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. $\operatorname{tr} e^{-\beta H^0} < \infty$, 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

$$\varepsilon_0 < \varepsilon_1 \leq \varepsilon_2 \leq \cdots \ . \tag{2}$$

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*

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

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

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

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

By the Feynman-Kac formula [2],

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

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

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

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

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

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

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

After some algebra, this yields

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

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

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

where we have substituted

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

$\lambda_B = \hbar\sqrt{2\pi\beta/m}$ 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 equations (1.14) and (1.31) of [2])

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

where m_d and n_d depend only on the dimension d,

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

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

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

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 $\mathbf{r} = (x_1,\dots,x_d)$, we find

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

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

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

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

$$\mathrm{tr}\, e^{-\beta H^0} \leq e^{-\beta(V_m - V_0 \ln 2)} \left(\mathrm{tr}\, e^{-\beta h^0}\right)^d \ . \tag{18}$$

Let λ_n, $n \geq 0$, be the eigenvalues of h^0 in increasing order. From Theorem 7.4 of [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

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

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

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

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

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

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 equation (20), and shows an exponential growth with the energy. This is origin of the divergence of the trace for small β in the case of logarithmically increasing potentials.

3 Free Bose gas in a deep trap

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

$$H_N^0 = \sum_{i=1}^{N} H^0(i) = T_N + \sum_{i=1}^{N} V(\mathbf{r}_i) \qquad T_N = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\Delta_i \ . \tag{22}$$

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*

$$\lim_{N\to\infty} e^{\beta N \varepsilon_0} Z[\beta H_N^0] \equiv e^{-\beta F_0(\beta)} \tag{23}$$

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

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

$$Z[\beta H_N^0] = \sum_{\{n_j\}:\sum n_j = N} e^{-\beta\sum n_j\varepsilon_j} = \sum_{N'=0}^{N} e^{-\beta(N-N')\varepsilon_0} \sum_{\{n_j\}_{j>0}:\sum n_j = N'} e^{-\beta\sum n_j \varepsilon_j} \ . \tag{24}$$

Therefore

$$e^{\beta N\varepsilon_0} Z[\beta H_N^0] = \sum_{\{n_j\}_{j>0}:\sum n_j \leq N} e^{-\beta\sum n_j(\varepsilon_j - \varepsilon_0)} \ , \tag{25}$$

so that

$$\begin{aligned} \lim_{N\to\infty} e^{\beta N\varepsilon_0} Z[\beta H_N^0] &= \sum_{\{n_j\}_{j>0}:\sum n_j < \infty} e^{-\beta\sum n_j(\varepsilon_j-\varepsilon_0)} \\ &= \prod_{j=1}^{\infty}\sum_{n_j=0}^{\infty} e^{-\beta n_j(\varepsilon_j-\varepsilon_0)} = \prod_{j=1}^{\infty}\frac{1}{1-e^{-\beta(\varepsilon_j-\varepsilon_0)}} \end{aligned} \tag{26}$$

and

$$\beta F_0(\beta) = \sum_{j=1}^{\infty} \ln(1 - e^{-\beta(\varepsilon_j - \varepsilon_0)}) \ . \tag{27}$$

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 $n \geq N$. Then

$$\begin{aligned}\sum_{n=N}^\infty |\ln(1-a_n)| &= \sum_{n=N}^\infty |\sum_{l=1}^\infty \frac{a_n^l}{l}| \leq \sum_{n=N}^\infty \sum_{l=1}^\infty \frac{|a_n|^l}{l} \\ &= \sum_{n=N}^\infty |a_n| \sum_{l=1}^\infty \frac{|a_n|^{l-1}}{l} \leq 2\ln 2 \sum_{n=N}^\infty |a_n| < \infty\end{aligned}$$

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 $z \in \mathbb{C}$, $\mathrm{Re}\, z > 0$. 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 $\mathrm{Re}\, z \geq \epsilon$. 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 equation (23). The total free energy of the gas is

$$-\beta^{-1} \ln Z[\beta H_N^0] = N\varepsilon_0 + F_0(\beta) + o(1) \; . \tag{28}$$

Analyticity of F_0 implies that there is no phase transition. On the other hand, the free energy per particle of the infinite system is ε_0 at any temperature, so 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 equation (24),

$$P_{\beta H_N^0}(N' = 0) = \frac{e^{-\beta N \varepsilon_0}}{Z[\beta H_N^0]} \to e^{\beta F_0(\beta)} \quad \text{as} \quad N \to \infty \tag{29}$$

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

$$P_{\beta H_N^0}(N' \geq m) = P_{\beta H_N^0}(N' = 0) \sum_{\{n_j\}_{j>0}: m \leq \sum n_j \leq N} e^{-\beta \sum n_j(\varepsilon_j - \varepsilon_0)} \ . \tag{30}$$

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

$$P_{\beta H_N^0}(N' \geq m) \geq P_{\beta H_N^0}(N' = 0) e^{-\beta m(\varepsilon_1 - \varepsilon_0)} \ . \tag{31}$$

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

$$\liminf_{N \to \infty} \frac{1}{a_N} \ln P_{\beta H_N^0}(N' \geq a_N) \geq -\beta(\varepsilon_1 - \varepsilon_0) \ . \tag{32}$$

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

$$\begin{aligned} P_{\beta H_N^0}(N' &\geq m) \\ &= P_{\beta H_N^0}(N' = 0) \sum_{N'=m}^{N} e^{-\beta \mu N'} \sum_{\{n_j\}_{j>0}: \sum n_j = N'} e^{-\beta \sum n_j(\varepsilon_j - \varepsilon_0 - \mu)} \\ &\leq P_{\beta H_N^0}(N' = 0)\ e^{-\beta \mu m} \prod_{j=1}^{\infty} \frac{1}{1 - e^{-\beta(\varepsilon_j - \varepsilon_0 - \mu)}} \\ &= P_{\beta H_N^0}(N' = 0)\ Q(\beta, \mu)\ e^{-\beta \mu m} \end{aligned} \tag{33}$$

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 $m = a_N \to \infty$,

$$\limsup_{N \to \infty} \frac{1}{a_N} \ln P_{\beta H_N^0}(N' \geq a_N) \leq -\beta \mu \ . \tag{34}$$

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 (32) is an upper bound as well, and (32) and (34) together yield

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

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

By the Borel-Cantelli lemma, inequality (33) 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

$$\langle N' \rangle_{\beta H_N^0} \leq \frac{P_{\beta H_N^0}(N' = 0)\; Q(\beta, \mu)}{(1 - e^{-\beta\mu})^2} \tag{36}$$

so that

$$\lim_{N\to\infty} \langle N' \rangle_{\beta H_N^0} \leq \frac{1}{Q(\beta, 0)} \inf_{0<\mu<\varepsilon_1-\varepsilon_0} \frac{Q(\beta, \mu)}{(1 - \exp -\beta\mu)^2} \,. \tag{37}$$

Let us summarize the results of this section:

Theorem 1 *N noninteracting bosons in a deep trap with eigenenergies $\varepsilon_0 < \varepsilon_1 \leq \cdots$ have a free energy $N\varepsilon_0 + F_0(\beta) + o(1)$, where F_0 is an analytic function of β 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.*

4 Condensation of interacting bosons

4.1 The order we are looking for

Due to the pioneering work of Penrose [4] and subsequent papers by Penrose and Onsager [5] and Yang [6], 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, σ_1, and means that the largest eigenvalue of σ_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 σ_1, was demonstrated in [5]. 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 [6], let σ be a density matrix, i.e., a positive operator of trace 1 acting in $\mathcal{H}^N$, where $\mathcal{H}$ is a one-particle separable

Hilbert space. We suppose σ to be invariant under the permutations of the particles. The associated one-particle reduced density matrix, σ_1, is a positive operator of trace N in $\mathcal{H}$, obtained by taking the sum of the partial traces of σ over the $N-1$- particle subspaces: If $\{\varphi_n\}_{n=0}^\infty$ is any orthonormal basis in $\mathcal{H}$ and ϕ and ψ are any elements of $\mathcal{H}$ then

$$\begin{aligned}(\phi,\sigma_1\psi) &\equiv \sum_{j=1}^N \sum_{\{i_k\}_{k\neq j}} (\varphi_{i_1}\cdots\varphi_{i_{j-1}}\phi\varphi_{i_{j+1}}\cdots\varphi_{i_N}, \sigma\,\varphi_{i_1}\cdots\varphi_{i_{j-1}}\psi\varphi_{i_{j+1}}\cdots\varphi_{i_N}) \\ &= N\sum_{i_2,\ldots,i_N}(\phi\varphi_{i_2}\cdots\varphi_{i_N},\sigma\,\psi\varphi_{i_2}\cdots\varphi_{i_N}) \qquad (38)\end{aligned}$$

because of the permutation-invariance of σ. In (38) the summation over each i_k is unrestricted and the matrix elements of σ are taken with simple (non-symmetrized) tensor products ($\otimes$ omitted).

Let φ_0 be any normalized element of $\mathcal{H}$. We define the *mean* (with respect to σ) *number of particles occupying* φ_0 as follows. We complete φ_0 into an orthonormal basis $\{\varphi_n\}_{n=0}^\infty$ of $\mathcal{H}$. In $\mathcal{H}^N$ we use the product basis

$$\{\Phi_{\mathbf{i}} = \varphi_{i_1}\otimes\cdots\otimes\varphi_{i_N} | \mathbf{i}=(i_1,\cdots,i_N)\in\mathbb{N}^N\} \ . \qquad (39)$$

To φ_0 and $\Phi_{\mathbf{i}}$ we assign

$$n[\varphi_0](\mathbf{i}) \equiv \sum_{j=1}^N |(\varphi_0,\varphi_{i_j})|^2 = \sum_j \delta_{i_j,0} \ , \qquad (40)$$

which is the number of particles in the state φ_0 among N particles occupying the states $\varphi_{i_1},\ldots,\varphi_{i_N}$, respectively. One can interprete $(\Phi_{\mathbf{i}},\sigma\Phi_{\mathbf{i}})$ as the probability of $\Phi_{\mathbf{i}}$. Then $n[\varphi_0](\mathbf{i})$ is a random variable whose mean value with respect to σ is

$$\begin{aligned}\langle n[\varphi_0]\rangle_\sigma &\equiv \operatorname{Tr} n[\varphi_0]\sigma = \sum_{i_1,\ldots,i_N}\sum_{j=1}^N \delta_{i_j,0}(\Phi_{\mathbf{i}},\sigma\Phi_{\mathbf{i}}) \\ &= \sum_{j=1}^N\sum_{i_j}\delta_{i_j,0}\sum_{\{i_k\}_{k\neq j}}(\Phi_{\mathbf{i}},\sigma\Phi_{\mathbf{i}}) = \frac{1}{N}\sum_{j=1}^N\sum_{i_j}\delta_{i_j,0}(\varphi_{i_j},\sigma_1\varphi_{i_j}) \\ &= \sum_{i=0}^\infty \delta_{i,0}(\varphi_i,\sigma_1\varphi_i) = (\varphi_0,\sigma_1\varphi_0) \ , \qquad (41)\end{aligned}$$

an intrinsic quantity independent of the basis. Reading equation (41) 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* φ_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* $\varphi_0 \in \mathcal{H}$ *(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, ψ_{σ_1}, of σ_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 ψ_{σ_1} can serve for proving BEC. We can even find an infinite orthogonal family of vectors, all having a nonvanishing asymptotic overlap with ψ_{σ_1}. One can speak about a generalized condensation [7] only when the occupation of more than one eigenstate of σ_1 becomes asymptotically divergent. In the noninteracting gas ψ_{σ_1} is just the ground state of the one-body Hamiltonian.

The homogeneous gas represents a particular case. Namely, $\psi_{\sigma_1}(\mathbf{r}) = \psi^L_{\mathbf{k}=0}(\mathbf{r}) \equiv 1/L^{d/2}$ 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 σ_1 is diagonal in momentum representation, therefore $\psi^L_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/L^{d/2}$ 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 $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is a translation invariant positive symmetric function) and by the Perron-Frobenius theorem 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 [8]).

In the case of a trapped gas we do not know the dominant eigenvector of σ_1. However, we can carry through the proof by the use of the ground state of H^0.

4.2 Interacting bosons in a deep trap

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

$$H_N = H_N^0 + U_N \ . \tag{42}$$

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 and the probability according to the canonical Gibbs measure will be denoted by $Z[\beta H_N]$ and $P_{\beta H_N}$, respectively. We want to prove the *persistence* of BEC in the presence of interaction, that is, a sort of continuity of the low-temperature phase as U_N increases from zero to some finite strength. This will be achieved by proving condensation into the ground state of H^0, i.e., macroscopic occupation of φ_0, defined by $H^0\varphi_0 = \varepsilon_0\varphi_0$.

The density matrix is

$$\sigma = P_N^+ e^{-\beta H_N}/Z[\beta H_N] \tag{43}$$

where $P_N^+ = (1/N!)\sum_{\pi\in S_N} \pi$ is the orthogonal projection to the symmetric subspace of $\mathcal{H}^N$ and $Z[\beta H_N] = \operatorname{Tr} P_N^+ e^{-\beta H_N}$.We cannot expect, and will not obtain, a 100% condensation in φ_0, as in the noninteracting case, because the overlap $(\varphi_0, \psi_{\sigma_1})$ must decrease with the interaction strength. (The 100% condensation [1] into $\phi_{\rm GP}$, the minimizer of the Gross-Pitaevskii functional, found for the ground state of the interacting gas in the dilute limit, means that $(\phi_{\rm GP}, \psi_{\sigma_1}) \to 1$ as $N \to \infty$. In this case $\sigma = |\Psi\rangle\langle\Psi|$, where Ψ is the unknown ground state.)

In the next theorem we use the basis of the H^0 eigenstates, given by $H^0\varphi_j = \varepsilon_j\varphi_j$, and the associated symmetrized and normalized products, cf (39),

$$\Psi_{\mathbf{i}} = P_N^+\Phi_{\mathbf{i}}/\|P_N^+\Phi_{\mathbf{i}}\| \tag{44}$$

for $\mathbf{i} = (i_1 \le i_2 \le \cdots \le i_N)$. In particular, for $i_j = 0$, all j, $\Psi_{\mathbf{i}} = \Phi_0 = \otimes_{i=1}^N \varphi_0(\mathbf{r}_i)$, the ground state of H_N^0.

Theorem 2 *Suppose that*

$$\delta \equiv \limsup_{N\to\infty} \frac{1}{N}[-\inf U_N + (\Phi_0, U_N\Phi_0)] < \varepsilon_1 - \varepsilon_0 \ . \tag{45}$$

Then for any $d \geq 1$, at any $\beta > 0$, φ_0 is macroscopically occupied. The fraction of particles in φ_0 tends to 1 as δ tends to 0.

Proof. Let $N'(\mathbf{i}) = N - n[\varphi_0](\mathbf{i})$. The bounds (33) and (45) and the convexity of the exponential imply

$$\begin{aligned}
P_{\beta H_N}(N' \geq m) &= \sum_{\mathbf{i}:N'(\mathbf{i})\geq m} (\Psi_{\mathbf{i}}, e^{-\beta H_N}\Psi_{\mathbf{i}}) / \sum_{\mathbf{i}} (\Psi_{\mathbf{i}}, e^{-\beta H_N}\Psi_{\mathbf{i}}) \\
&\leq \frac{e^{-\beta \inf U_N} Z[\beta H_N^0]}{(\Phi_0, e^{-\beta H_N}\Phi_0)} P_{\beta H_N^0}(N' \geq m) \\
&\leq e^{\beta[-\inf U_N + (\Phi_0, U_N \Phi_0)]} \frac{P_{\beta H_N^0}(N' \geq m)}{P_{\beta H_N^0}(N' = 0)} \\
&\leq e^{\beta\delta' N}\, Q(\beta,\mu) e^{-\beta\mu m} \qquad (46)
\end{aligned}$$

for any $\delta' > \delta$, if N is large enough. Choosing, e.g., $m = \sqrt{\frac{\delta'}{\varepsilon_1 - \varepsilon_0}} N$ and $\sqrt{\delta'(\varepsilon_1 - \varepsilon_0)} < \mu < \varepsilon_1 - \varepsilon_0$, letting $N \to \infty$ and then $\delta' \to \delta$, we find

$$\lim_{N\to\infty} P_{\beta H_N} \left(\frac{n[\varphi_0]}{N} \geq 1 - \sqrt{\frac{\delta}{\varepsilon_1 - \varepsilon_0}} \right) = 1 \ . \qquad (47)$$

As a consequence,

$$\lim_{N\to\infty} \frac{1}{N} \langle n[\varphi_0] \rangle_{\beta H_N} \geq 1 - \sqrt{\frac{\delta}{\varepsilon_1 - \varepsilon_0}} \ , \qquad (48)$$

which proves the theorem.

As an example, we shall consider only translation invariant pair interactions. The interaction energy is then

$$U_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{1 \leq i < j \leq N} u_N(\mathbf{r}_i - \mathbf{r}_j) \ . \qquad (49)$$

To comply with condition (45), the pair interaction must depend on N. The simplest example is a mean-field interaction of the form $u_N = (1/N)u$, where u is bounded below and

$$\int\int \varphi_0(\mathbf{x})^2 u(\mathbf{x} - \mathbf{y}) \varphi_0(\mathbf{y})^2 \, d\mathbf{x}\, d\mathbf{y} < \infty \ , \qquad (50)$$

and both $-\inf u$ and the integral above are small enough. Such an interaction effectively scales the temperature down to zero.More interesting examples are provided by scaled interactions.

Corollary 4.2 *Let $u : \mathbb{R}^d \to \mathbb{R}$ be an integrable nonnegative function. Suppose we are given some $a_0 > 0$ and two positive sequences a_N and b_N satisfying the condition*

$$\limsup_{N\to\infty} \; b_N \left(\frac{a_N}{a_0}\right)^d N < 2\frac{\varepsilon_1 - \varepsilon_0}{\|u\|_1 \|\varphi_0^4\|_1} \; . \tag{51}$$

Then there is Bose-Einstein condensation for the interaction

$$u_N(\mathbf{x}) = b_N u(a_0\mathbf{x}/a_N) \;\; : \tag{52}$$

φ_0 is macroscopically occupied for any $\beta > 0$.

Proof.

$$\begin{aligned}(\Phi_0, U_N\Phi_0) &= \binom{N}{2} \int \varphi_0(\mathbf{x})^2 u_N(\mathbf{x}-\mathbf{y})\varphi_0(\mathbf{y})^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} \\ &= \binom{N}{2} b_N \left(\frac{a_N}{a_0}\right)^d (2\pi)^{d/2} \int \hat{u}(a_N\mathbf{q}/a_0)|\widehat{\varphi_0^2}(\mathbf{q})|^2 \,\mathrm{d}\mathbf{q} \\ &\le \binom{N}{2} b_N \left(\frac{a_N}{a_0}\right)^d \|u\|_1 \|\varphi_0^4\|_1 \; ,\end{aligned} \tag{53}$$

and $-\inf U_N \le 0$. Comparison with (45) yields the result.

Remarks.

1. The scaling (52) with condition (51) implies

$$\|u_N\|_1 = b_N \left(\frac{a_N}{a_0}\right)^d \|u\|_1 < \frac{2}{N}\frac{\varepsilon_1 - \varepsilon_0}{\|\varphi_0^4\|_1} \; . \tag{54}$$

2. If a_N is constant, we obtain the mean-field interaction. If a_N is strictly monotonous or, at least, the sequence has no repeated values, a_N can be inverted and, hence, b_N may depend on N only via a_N, $b_N = f(a_0/a_N)$. For example, $a_0/a_N = N^\eta$, $b_N = (a_0/a_N)^{d-\frac{1}{\eta}}$ and $\|u\|_1 < 2(\varepsilon_1 - \varepsilon_0)/\|\varphi_0^4\|_1$ satisfy (51).

3. If a_0 is the scattering length of u and $b_N = (a_0/a_N)^2$ then a_N is the scattering length of u_N. To see this, we recall (cf. [9]) 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 energy bound state. Then the Schrödinger equation written for zero energy,

$$-\frac{\hbar^2}{2m}\Delta\phi(\mathbf{x}) + V(\mathbf{x})\phi(\mathbf{x}) = 0 \tag{55}$$

has a (up to constant multipliers) unique spherical sign-keeping solution, ϕ_0. If $r = |\mathbf{x}| > R_0$, the range of the potential, this solution reads

$$\phi_0(\mathbf{x}) = \begin{cases} 1 - (a/r)^{d-2} & \text{if } d \neq 2 \\ \ln(r/a) & \text{if } d = 2 \end{cases} \tag{56}$$

with some $a \leq R_0$. We call a the scattering length of V and ϕ_0 the defining solution. To obtain the scattering length of a pair interaction u one has to solve (55) 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 [9].

Suppose now that the scattering length of u is a_0. What is the scattering length of u_N, given by (52)? 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 equations (55) and (56) it is easily seen that the defining solutions of u and

$$u_a(\mathbf{x}) = (a_0/a)^2 u(a_0\mathbf{x}/a) \tag{57}$$

are related by scaling, $\phi_0[u_a](\mathbf{x}) = \phi_0[u](a_0\mathbf{x}/a)$, and therefore the scattering length of u_a is a.

4. The bound (54), together with $u_N \geq 0$, implies that the scattering length of u_N tends to zero as $N \to \infty$ 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 one dimension (54) alone would suffice, however, in higher dimensions $u_N \geq 0$ is essential. Indeed, in two and three dimensions with a_N tending to zero and b_N chosen so that the bound (51) 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 [10]. However, it turns out that for $u_N \geq 0$ one can only obtain the trivial extension (cf. Theorems 1.2.5 and 5.5 of [10]). The result of the theorem and its corollary can be nontrivial because the scattering length vanishes in conjunction with a diverging particle number.

5. In three dimensions the Gross-Pitaevskii scaling limit is obtained by fixing Na, where a is the scattering length of the pair interaction, while $N \to \infty$. To show BEC, we choose $b_N = (a_0/a_N)^2$, so that $u_N = u_{a_N}$, and $a_N = a_0/N$. Then condition (51) reads $\|u\|_1 < 2(\varepsilon_1 - \varepsilon_0)/\|\varphi_0^4\|_1$. Observe that $\|u_{a_N}\|_1 = N^{-1}\|u\|_1$ for GP scaling in three dimensions.

6. In two dimensions the scaling described in the corollary cannot be realized with a_N being the scattering length of u_N. In general,

$$u_N(\mathbf{x}) = b_N \left(\frac{a_N}{a_0}\right)^2 u_{a_N}(\mathbf{x}) < cN^{-1}(a_0/a_N)^{d-2} u_{a_N}(\mathbf{x}) \tag{58}$$

where c is the constant on the right-hand side of (51) and u_{a_N}, defined by (57), has scattering length a_N. In particular, in two dimensions $u_N < (c/N)u_{a_N}$. Because for $u \geq 0$ the scattering length of λu increases with $\lambda > 0$, the scattering length of any admissible u_N is smaller than a_N. If $a_N \to 0$, this holds true also in one dimension. We note that in two dimensions $\|u_a\|_1 = \|u\|_1$, independently of a. The Gross-Pitaevskii scaling limit for a_N in two dimensions corresponds to fixing $g = 4\pi N/\ln(a_0^2 N/a_N^2)$ (cf. [9], [1]). Then condition (51) holds true if

$$b_N < \frac{2\pi c}{g}\left(\ln \frac{a_0}{a_N}\right)^{-1}\left(\frac{a_0}{a_N}\right)^2 .$$

For bosons in a locally bounded potential trap scaling of a nonnegative interaction is unavoidable in order that condensation takes place into a fixed φ_0, independent of N: Since φ_0 is exponentially localized, particles in φ_0 are confined in a box of side 2ℓ where ℓ is the localization length. An unscaled nonnegative interaction would push the particles outside this box and, hence, out of φ_0. 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.

Finally, condensation into a fixed state, as described by the theorem, implies that for increasing N, ψ_{σ_1} has an $O(1)$ overlap with this state and, hence, it converges in $\mathcal{H}$ as N tends to infinity, at least on a subsequence.

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