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Validity of the Hohenberg Theorem for a Generalized Bose-Einstein Condensation in Two Dimensions

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Several authors have considered the possibility of a generalized Bose-Einstein condensation (BEC) in which a band of low states is occupied so that the total occupation number is macroscopic, even if the occupation number of each state is not extensive. The Hohenberg theorem (HT) states that there is no BEC into a single state in 2D; we consider its validity for the case of a generalized condensation and find that, under certain conditions, the HT does not *forbid a BEC in 2D. We discuss whether this situation actually occurs in any theoretical model system.*

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1. INTRODUCTION

The Hohenberg theorem[1] (HT) provides the general statement that Bose-Einstein condensation (BEC) cannot occur in a two-dimensional system. In this analysis a condensation implies extensive occupation of a single state of the system, that is, a density of particles of order N/V, (where N is the number of particles in the system and V the volume of the system) in the thermodynamic limit. Recently however there has been renewed interest in the possibility of a "smeared," "fragmented," or "generalized" BEC, in which some finite band of states, rather than a single state, is occupied. Nozières and Saint James[2] and more recently Nozières[3], using a Hartree-Fock approximation at zero temperature, showed that repulsive interactions favor single-state occupancy. There have been earlier discussions of generalized BEC in the literature, for example, by Girardeau[4], Luban[5]

and Van den Berg *et al*[6]. Van den Berg and Lewis[7] have even presented a non-interacting model in which an extensive BEC occurs in each state of a band of momentum states. Ho and Yip[8] discuss fragmentation in a recent paper and claim that the spin-1 Bose gas[9] is an example of the occurrence of this phenomenon.

In two dimensions (2D), where the HT applies, there is no single-state BEC, but there is a Kosterlitz-Thouless[10] transition to a superfluid state. However, one can ask whether there could be a generalized transition, and, if so, whether it is related to the KT transition, or whether the generalized transition is also forbidden by the HT.

If the generalized BEC is to be possible, we might envision different forms of it. One possibility (which we call "fragmentation") is that each of a finite number of states is extensively occupied (occupation proportional to N) and that the sum of all the particles in such a condensate is still of order N. Another interesting possibility (here termed "smearing") is that no single state is extensively occupied, but that the sum of the occupation numbers of all the states in a band is extensive. For example, one might have $O(\sqrt{N})$ states each occupied by $O(\sqrt{N})$ particles so that the total number of particles is of order N. The question is whether the HT forbids either of these kinds of generalized condensation in 2D.

The generalized condensation studied in Ref. [7] occurs in 2D, which seems to violate the HT, but there are some subtle aspects that need to be considered to see how this case fits into the general picture. The example given there consists of particles moving freely in one dimension and bound harmonically in the other. The condensation occurs in the lowest harmonic band of states. In a similar problem, free particles trapped in a 2D harmonic potential are known to have a BEC, but this arises because there is a "loophole" in the HT, due to of the inhomogeneous potential. One can show[11] that the HT does indeed apply to the case of trapped inhomogenous fluids, but that its application requires that the particle density be everywhere bounded. When Bose condensed, the ideal gas in a trap has an integrable singularity in its density in the thermodynamic limit, and thus does not fall under the conditions covered by the HT. However, as soon as repulsive hard-core interactions are turned on, this singularity disappears and the HT applies.[11] Similarly, the example of Ref. [7] is not a case of a violation of the HT because of fragmenting of the condensate, but rather a case where the HT does not apply because one has an ideal gas in a trap.

The situation we will consider here is a homogeneous system (particles in a box) in which we suppose that a generalized BEC occurs as mentioned above, namely, a narrow band of momentum states occupied either extensively or non-extensively, but with the sum of their occupation numbers

extensive.

2. DERIVATION

We consider a homogenous system of N particles. We follow the derivation of the Hohenberg theorem due to Chester.[12] Start with the Bogoliubov inequality given by

$$\left\langle \frac{1}{2}\left\{A, A^{\dagger}\right\}\right\rangle \geqslant \frac{kT\left|\langle[C, A]\rangle\right|^{2}}{\langle[[C, H], C^{\dagger}]\rangle}, \tag{1}$$

where $\langle ...\rangle$ means thermal average, A and C are operators, and H is the system Hamiltonian. Choose $A = a_{\mathbf{p}} a^{\dagger}_{\mathbf{p+k}}$, and $C = \sum_{\mathbf{q}} a^{\dagger}_{\mathbf{q}} a_{\mathbf{q+p}}$, where $a^{\dagger}_{\mathbf{p}}$ creates a particle with momentum $\mathbf{p}$. C, being the Fourier transform of the density operator, commutes with the interaction potential energy in H, so we need only to consider commutators with the kinetic energy. Upon carrying out these commutators we find

$$\begin{aligned}
\left\langle \frac{1}{2}\left\{A, A^{\dagger}\right\}\right\rangle &= n_{\mathbf{p}} n_{\mathbf{p+k}} + \frac{1}{2}(n_{\mathbf{p}} + n_{\mathbf{k}}) + \delta_{\mathbf{k},0}(n_{\mathbf{p}} + 1), && (2)\\
\langle[C, A]\rangle &= n_{\mathbf{p}} - n_{\mathbf{p+k}}, && (3)\\
\left\langle \left[[C, H], C^{\dagger}\right]\right\rangle &= \frac{\hbar^2}{2m}\sum_{\mathbf{q}}\left[(\mathbf{k}+\mathbf{q})^2 + (\mathbf{k}-\mathbf{q})^2 - 2\mathbf{q}^2\right] n_{\mathbf{q}} \\
&= \frac{\hbar^2 k^2}{m}\sum_{\mathbf{q}} n_{\mathbf{q}} = N\frac{\hbar^2 k^2}{m}, && (4)
\end{aligned}$$

where $n_{\mathbf{p}}$ is the thermal average number of particles in state $\mathbf{p}$. The inequality becomes

$$n_{\mathbf{p}} n_{\mathbf{p+k}} + \frac{1}{2}(n_{\mathbf{p}} + n_{\mathbf{k}}) + \delta_{\mathbf{k},0}(n_{\mathbf{p}} + 1) \geqslant \frac{kTm}{N\hbar^2 k^2}(n_{\mathbf{p}} - n_{\mathbf{p+k}})^2. \tag{5}$$

We assume that there are M_c condensed states (our generalized condensate band) containing N_0 particles with $N_0 = O(N)$, and that these states are clustered in momentum space around $\mathbf{k} = 0$ in a circle out to radius p_c. The non-condensed states are in the region beyond p_c. We assume that the condensed states each have occupation that, while not necessarily extensive, still greatly exceeds that of any non-condensed state. We have then $\sum_{p<p_c} 1 = M_c, \quad \sum_{p<p_c} n_{\mathbf{p}} = N_0$. If we change the sum to an integral, the first of these equations becomes

$$M_c = \sum_{\mathbf{p}=0}^{p_c} 1 = \frac{L^2}{2\pi}\frac{p_c^2}{2}, \tag{6}$$

where L is the dimension of the box and $n = N/L^2$ is the density. Thus

$$p_c = c_1 \left(\frac{M_c}{N}\right)^{1/2} n^{1/2}, \tag{7}$$

where c_1 is a constant of order unity.

Sum both sides of Eq.(5) on $\mathbf{k}$ over the range $2p_c < k < p_m$, where the upper limit k_m satisfies $k_m = c_2 n^{1/2}$ with c_2 a constant. Below we will see why we take the minimum k value as twice p_c rather than just p_c. We have

$$n_{\mathbf{p}} \sum_{\mathbf{k}} n_{\mathbf{p}+\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} (n_{\mathbf{p}} + n_{\mathbf{k}}) \geqslant \frac{kTm}{N\hbar^2} \sum_{\mathbf{k}} \frac{(n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{k}})^2}{k^2}. \tag{8}$$

We assume that $\mathbf{p}$ is in the range of condensed states so that the second term in the second sum on the left is much smaller than the first and can be neglected. The remaining term in that sum is

$$n_{\mathbf{p}} \sum_{\mathbf{k}} 1 = \frac{L^2}{2\pi} \int_{2p_c}^{p_m} dk k = n_{\mathbf{p}} \frac{N}{n(4\pi)} (p_m^2 - 4p_c^2) = N n_{\mathbf{p}} \gamma, \tag{9}$$

where $\gamma = (c_2 - 4c_1 \frac{M_c}{N})/(4\pi)$ is a constant of order unity. The first sum on the left of Eq.(8) is over only a portion of momentum space and results in a fraction of the total particle number. Increasing the sum to the full number of particles just amplifies the inequality. We then can write $n_{\mathbf{p}} N(1+\gamma)$ for the left side.

The sum on the right side of Eq.(8) has the vector $\mathbf{k} + \mathbf{p}$ extending outside the condensate range because of the restriction that $k > 2p_c$. If we had defined the minimum value of k as just p_c then, by putting $\mathbf{k}$ and $\mathbf{p}$ in opposite directions, the sum could extend back into the condensate circle. As it is we can neglect $n_{\mathbf{p}+\mathbf{k}}$ relative to $n_{\mathbf{p}}$ on the right side of the equation to give simply $n_{\mathbf{p}}^2 \sum_{\mathbf{k}} 1/k^2$. The sum is evaluated by doing the appropriate integral:

$$\sum_{\mathbf{k}} \frac{1}{k^2} = \frac{N}{n(2\pi)} \int_{2p_c}^{p_m} dk \frac{1}{k} = c_3 \frac{N}{n} \ln\left(\frac{p_m}{2p_c}\right). \tag{10}$$

The result is

$$n_{\mathbf{p}} N(1+\gamma) \geqslant n_{\mathbf{p}}^2 \frac{kTm}{N\hbar^2} c_3 \frac{N}{n} \ln\left(\frac{p_m}{2p_c}\right) \tag{11}$$

or

$$\frac{n_{\mathbf{p}}}{N} \leqslant \frac{\hbar^2 n}{mkTc_3} \frac{1+\gamma}{\ln\left(\frac{p_m}{2p_c}\right)}. \tag{12}$$

Now sum this over all states in the condensate circle to give

$$\frac{N_0}{N} \leqslant \frac{\hbar^2 n}{mkTc_3} \frac{(1+\gamma)}{\ln\left(c_4\sqrt{\frac{N}{M_c}}\right)} M_c. \tag{13}$$

where we have used the fact that

$$\frac{p_m}{2p_c} = \frac{c_2\sqrt{n}}{2c_1\sqrt{n\frac{M_c}{N}}} = c_4\sqrt{\frac{N}{M_c}}. \tag{14}$$

If $M_c = 1$, as in the usual case, then, in the thermodynamic limit, the right side goes to zero as $1/\ln(N)$ and there is no BEC. However, if $M_c = O(N^\nu)$, where ν is any power not equal to zero, then the inequality becomes

$$\frac{N_0}{N} \leqslant \frac{\hbar^2 n}{mkT} \frac{N^\nu}{\ln\left(N^{(1-\nu)/2}\right)}. \tag{15}$$

Now the right side *diverges* as $N \to \infty$. For example, if $\nu = \frac{1}{2}$ then the right side is of order $\sqrt{N}/\ln(N)$, which clearly diverges. In this case we can no longer rule out the possibility of BEC by this argument.

3. DISCUSSION

Our derivation does not *prove* that BEC actually happens in a generalized mode. Moreover, it also does not insure that there might not be *another* more powerful derivation of the HT that outlaws a generalized condensation in 2D. In the case of a fragmented condensate (as in Ref. [7]), one can have only a finite number, M_c, of states each containing $O(N)$ particles so that M_c is $O(1)$ and *there can be no fragmented BEC in a 2D homogeneous system.* The fragmented case of Ref. [7] is "tainted" by the fact that the HT conditions for the inhomgeneous case are violated by a divergent density of particles so that it is not a counter-example to the HT case that we discuss in this paper. A 2D version of the spin-1 gas, claimed in Ref. [8] to be an example of fragmentation in 3D, would not fall directly under our derivation because it is a condensation in *spin* space, not in the momentum space of our derivation. (The spin-1 Bose system appears to be a case that violates the claim of Refs. [2] and [3] that a single-state BEC was favored over generalized BEC. However, that discussion was based on use of mean-field theory and the spin-1 system analyses go beyond mean-field approximations.)

On the other hand, the analysis above leaves open the possibility of a smeared BEC in 2D. In this case, $N^\nu(\nu < 1)$ states each containing only a

non-extensive number of particles constitute a condensate as a unit. Note that the width of this band of states, as given in Eq.(7), tends to zero as N increases, so one still gets a δ-function occupation in the thermodynamic limit.

A question yet to be answered is whether the KT transition is related in some way to a generalized BEC. The analysis of Popov[13] of the KT state at low temperature involves what he calls a "bare" condensate spread over a set of states up to some cut-off k_0. He says "the particles with momenta small compared with the faster particles behave like a condensate." However, it is not clear to us at this time whether this situation would qualify as a generalized condensate in the sense of our theorem above.

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