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Bose-Einstein condensation in real space

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We show how Bose-Einstein condensation (BEC) occurs not only in momentum space but also in coordinate (or real) space. Analogies between the isotherms of a van der Waals classical gas of extended (or finite-diameter) identical atoms and the point (or zero-diameter) particles of an ideal BE gas allow concluding that, in contrast with the classical case, the volume per particle vanishes in the pure BE condensate phase precisely because the boson diameters are zero. Thus a BE condensate forms in real space without exhibiting a liquid branch as does the classical gas.

Keywords: Bose-Einstein condensation; boson gas; van der Waals gas.

Mostramos cómo la condensación Bose-Einstein (BEC, por sus siglas en inglés) ocurre no solamente en el espacio de momentos sino también en el espacio de coordenadas (o real). Para ello empleamos la analogía entre las isotermas del gas clásico de van der Waals de átomos idénticos con diámetro finito y las del gas ideal cuántico de bosones puntuales (diámetro cero), que nos permite concluir, contrario a lo que sucede en el caso clásico, que el volumen por partícula de la fase condensada de BE se anula precisamente porque los bosones son puntuales. Así, el condensado de BE se forma en el espacio real sin exhibir la rama líquida del gas clásico.

Descriptores: Condensación Bose-Einstein; gas de bosones; gas de van der Waals.

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1. Introduction

Since its theoretical inception in 1925, and particularly its experimental observation in 1995 [1–3], Bose-Einstein condensation (BEC) has commanded much interest and research effort. Its proper discussion is essential in any elementary course in statistical or quantum mechanics. There it is viewed as the macroscopic manifestation of the quantum behavior of a many-particle system, not to speak of its many applications to superfluidity and superconductivity.

Nevertheless, several doubts remain as to the fundamental properties of this transition. It is sometimes said that the BEC in a perfect or ideal (*i.e.*, without interactions) boson gas is a condensation in momentum space *only*, and not in coordinate or real space like the condensation of vapor into liquid. For example: F. London [4] claims that "*. . . one may say that there is actually a condensation, but only in momentum space, and not in ordinary space, ...[where] no separation of phases is to be noticed.*" [5]. The same author speaks of bosons that "*. . . settle in some kind of order in momentum space even at the expense of order in ordinary space.*" Landau & Lifshitz [6] state that: "*The effect of concentrating the particles in the state* $\epsilon = 0$ *is often called 'BEC'. We must emphasize that at best one might perhaps talk about 'condensation in momentum space.' Actual condensation certainly does not take place in the gas.*" T.L. Hill [7] asserts that "*. . . As it is usually stated, the condensation occurs in momentum space rather than in coordinate space: the condensed phase consists of molecules with zero energy and momentum, and macroscopic de Broglie wavelength.*" Fetter & Walecka [8] say this: "*. . . The assembly is ordered in momentum space and not in coordinate space; this phenomenon is called BEC.*" B. Maraviglia [9] writes (freely translated) that "*. . . Superfluity results from the fact that the* ^4He *atoms, since they obey BE statistics, can condense not in position but in momentum space. . .* " F. Mandl [10] says "*. . . It differs from the condensation of a vapor into a liquid in that no spatial separation into phases with different properties occurs in BEC.*" Finally, D.A. McQuarrie [11] p. 176 concludes "*. . . Therefore the BEC is a first-order process. This is a very unusual first-order transition, however, since the condensed phase has no volume, and the system therefore has a uniform macroscopic density rather than the two different densities that are usually associated with first-order phase transitions. This is often interpreted by saying that the condensation occurs in momentum space rather than coordinate space,. . .* "

In this paper we argue, using a analogy with the well known van der Waals gas of point classical particles, that the BEC is a phase transition which occurs in the momentum *as well as in the real space* provided an external potential such as a gravitational field [12] or a magneto-optical trap is applied, bringing us in agreement with the assertions of other authors, *e.g.*, R. Becker [13], D. ter Haar [14], K. Huang [15] and D.L. Goodstein [16].

We first summarize in Sec. 2 the van der Waals theory of a classical gas and in Sec. 3 the Bose-Einstein condensation. In Sec. 4 we stress an analogy between the van der Waals gas in the limit of zero-diameter particles, and the ideal boson gas which by definition consists of point bosons. Section 5 contains conclusions.

2. Van der Waals gas

The van der Waals equation of state for a classical monatomic gas is

$$\left[P + a\left(\frac{N}{V}\right)^2\right](V - Nb) = Nk_BT, \tag{1}$$

where P is the pressure, V the volume, T the absolute temperature, N the number of atoms and k_B Boltzmann's constant. The effective "excluded volume" per particle [17] is

$$b = \frac{1}{2}\left(\frac{4}{3}\pi\sigma^3\right) = \frac{2}{3}\pi\sigma^3; \tag{2}$$

where σ is the diameter of each particle, thought of as a hard sphere. It is the reduction in the original volume per particle V/N due to finite-sized atoms, and was proposed by Clausius for an imperfect gas [17]. In 1873 van der Waals introduced a second correction term (see *e.g.*, Ref. 17) to the equation of state $PV = Nk_BT$ of an ideal gas to account for the attractive forces between molecules. In (1) the parameter a is given by

$$a \equiv -\frac{4\pi}{2}\int_\sigma^\infty u(r)r^2dr, \tag{3}$$

where $u(r) \leq 0$ is the attractive interaction potential between two atoms whose center-to-center separation is r.

On a $P - V$ phase diagram (1) exhibits the well-known isotherm loops signaling a vapor to liquid phase transition. One such loop (at a given T) is shown in Fig. 1 (left panel), where the horizontal plateau connecting points D and B is called the "Maxwell construction." Loops occur only for isotherms with $T < T_c$, where T_c is the critical point where both $(dP/dV)_T = 0$ (zero slope) and $(d^2P/dV^2)_T = 0$ (change of curvature). These two conditions along with (1) give

$$P_c = \frac{a}{27b^2}; \quad V_c = 3Nb; \quad T_c = \frac{8a}{27k_Bb} \tag{4}$$

for the critical pressure, volume and temperature.

3. Bose-Einstein condensation

For a quantum ideal gas in three dimensions

$$PV = \frac{2}{3}U, \tag{5}$$

where U is the internal energy, if a quadratic energy-momentum (or dispersion) relation holds for each particle [18]. If T_c is the BEC transition temperature below which there is

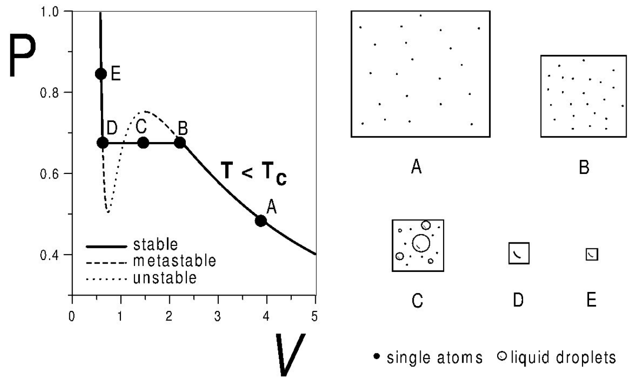

FIGURE 1. **Left**: Schematic sketch of a typical van der Waals isotherm below the critical temperature T_c in the pressure-volume plane (in arbitrary units) for a classical monatomic fluid of finite-sized atoms. The horizontal plateau DCB corresponds to Maxwell's construction, which separates "stable" from "metastable" states, the latter being separated by an "unstable" portion as shown. **Right**: illustration of how, as the volume of the system is reduced from points A to B to C and D along the chosen isotherm on the left, the vapor condenses first into several "droplets" of different sizes and finally into a single "self-bound" drop, D and E. All points such as E correspond to a sharp rise in pressure because the single drop at D is being compressed as volume is reduced.

macroscopic occupation in a given single quantum state (not mix up with critical temperature for a van der Waals gas), the internal energy for the ideal Bose gas for $T \leq T_c$ (or alternatively $V \leq V_c$ where V is the bosonic system volume and V_c the transition volume) is given in Ref. 15, Eq. (12.62). If we substitute Eqs. (12.55) into (12.62) of Ref. 15 we obtain

$$\frac{U(V,T)}{Nk_BT} = \frac{3}{2}\frac{\zeta(5/2)}{\zeta(3/2)}\left(\frac{T}{T_c}\right)^{3/2}, \quad \text{for all } V \leq V_c. \tag{6}$$

Here $\zeta(\sigma)$ is the Riemann-Zeta function. Thus, (5) and (6) give

$$P = \frac{2}{3}\frac{U}{V} = \frac{\zeta(5/2)}{\zeta(3/2)}\frac{Nk_BT}{V}\left(\frac{T}{T_c}\right)^{3/2}, \ (\text{for } V_c). \tag{7}$$

If we use for the thermal wavelength $\Lambda \equiv h/\sqrt{2\pi mk_BT}$ and Eq. (10.58) of Ref. 11, the condensate fraction for $T \leq T_c$ is

$$\frac{N_0(T)}{N} = 1 - \frac{\zeta(3/2)}{8\pi^{3/2}(\hbar^2/2m_Bk_BT)^{3/2}(N/V)}, \tag{8}$$

where $N_0(T)$ is the condensate particle number and N the total particle number. Using the fact that $N_0(T)$ is negligible compared with N when $T \geq T_c$, (8) leads to the well-known BEC T_c formula

$$T_c = \frac{\hbar^2}{2mk_B}\left[\frac{8\pi^{3/2}N/V}{\zeta(3/2)}\right]^{\frac{2}{3}} \simeq 3.313\frac{\hbar^2}{m_Bk_B}\left(\frac{N}{V}\right)^{\frac{2}{3}}, \tag{9}$$

since $\zeta(3/2) \simeq 2.612$. Alternatively, from (8) the critical volume V_c below which BEC appears at any temperature T is

$$V_c = \frac{(\hbar^2/2m_B k_B T)^{3/2} 8\pi^{3/2} N}{\zeta(3/2)}. \tag{10}$$

Combining (9) with (7) leaves the *volume-independent* pressure

$$P = \frac{2}{3}\frac{U}{V} = \frac{\zeta(5/2)}{\sqrt{(2\pi)^3}} \left(\frac{\sqrt{m_B}}{\hbar}\right)^3 (k_B T)^{5/2}$$
$$\simeq 0.0851 \left(\frac{\sqrt{m_B}}{\hbar}\right)^3 (k_B T)^{5/2}, \text{ for all } V \leq V_c, \tag{11}$$

which is consistent with Eq. (12.56) in Ref. 15, and where in the last step we used $\zeta(5/2) \simeq 1.341$. So, at constant temperature T if we reduce the volume below the value V_c given by (10), the pressure stays constant. This corresponds to the portion BCD of the isotherm depicted in the left panel of Fig. 2. The condensate fraction given by (8), combined with (10), simplifies to

$$\frac{N_0(T)}{N} = 1 - V/V_c \qquad \text{for all} \qquad V \leq V_c. \tag{12}$$

4. Zero volume a sign of real-space BEC

Imagine the ideal Bose gas to be in a cylinder with a movable piston. According to (11), if we push the piston in, decreasing the available volume below V_c, given by (10), at constant temperature T, the pressure remains constant. The piston can be pushed in at constant pressure until the two-phase region BCD of Fig. 2 vanishes, *i.e.*, until the condensate particle number N_0 equals the total number of particles N. Thus, at B the condensate just begins to appear and at D there is 100% condensate.

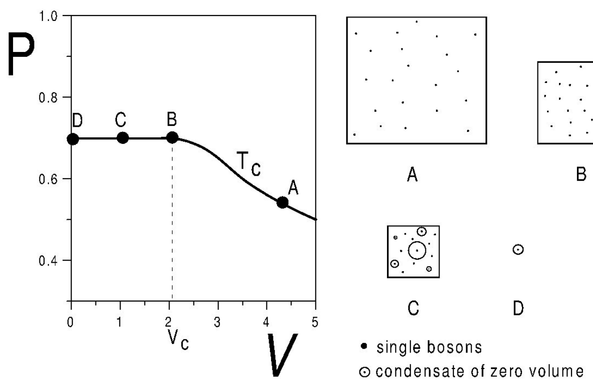

FIGURE 2. **Left**: schematic isotherm in the $P - V$ plane (in arbitrary units) for an ideal Bose gas at some fixed $T = T_c$ as given by (9). Being ideal, the gas consists of *zero*-diameter particles, *i.e.*, with zero-range interparticle repulsions. **Right**: illustration of how system behaves at different volumes marked as A, B, C and D on the isotherm, with circled dots of varying sizes denoting possibly different sized condensates of zero volume (since the bosons are point particles).

So, to have BEC in coordinate space the gas must be condensed in momentum space, *i.e.*, a macroscopic number of bosons must be in the ground state. The whole gas occupies zero volume only if the bosons are not moving with different speeds and directions. In the two-phase region, where $N \neq N_0 \neq 0$, the condensed phase consisting of several zero-diameter "droplets" with possibly different particle numbers does not occupy any volume at all. Fig. 2 shows how the volume becomes zero when the bosonic system is entirely condensed at point D; see also (12) when $N = N_0$. However, for a van der Waals fluid when the vapor is entirely condensed into liquid at D, Fig. 1, the volume cannot be zero because of finite particle sizes, and the pressure rises steeply to points E and beyond as the particles are further compressed against each other.

We have apparently fallen into a contradiction since $N = N_0$ usually applies to an ideal bosonic system at $T = 0$, and not to a system along a finite T isotherm. However, we note that in keeping with $N \to N_0$ for some $T \neq 0$, we approach the endpoint of the two-phase region where *all* the isotherms merge together, in particular the T_c isotherm with which we began as well as the $T = 0$ isotherm.

5. Conclusions

We have discussed a scenario in which, by analogy with a van der Waals gas of zero-diameter atoms, we illustrate how Bose-Einstein condensation (BEC) occurs not only in momentum space, *i.e.*, $N = N_0$, but also in real space if one applies a external potential such as a trap or a gravitational field. This vindicates the following claims in the largely textbook literature:

- R. Becker [13] p. 120, freely translated: "*...the number of atoms in the condensate phase, N_0, exhibits null volume...*"
- D. ter Haar [14] "*...one can also consider Einstein condensation to be a condensation in coordinate space.*"
- K. Huang [15] p. 290 "*...If we examine the equation of state alone, we discern no difference between the BEC and an ordinary gas-liquid condensation...*"
- D.L. Goodstein [16] p. 132 "*...condensation takes place in real as well as momentum space...*"

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