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Bose–Einstein condensation for general dispersion relations

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Abstract. Bose–Einstein condensation in an ideal (i.e. interactionless) boson gas can be studied analytically, at university-level statistical and solid state physics, in any positive dimensionality ($d > 0$) for identical bosons with any positive-exponent ($s > 0$) energy–momentum (i.e. dispersion) relation. Explicit formulae with arbitrary d/s are discussed for: the critical temperature (non-zero only if $d/s > 1$); the condensate fraction; the internal energy; and the constant-volume specific heat (found to possess a jump discontinuity only if $d/s > 2$). Classical results are recovered at sufficiently high temperatures. Applications to 'ordinary' Bose–Einstein condensation, as well as to photons, phonons, ferro- and antiferromagnetic magnons, and (very specially) to Cooper pairs in superconductivity, are mentioned.

1. Introduction

Experimental observations [1] reported in 1995 of Bose–Einstein condensation (BEC) in ultra-cold alkali-atom gas clouds, as well as the 1996 Nobel Prize [2] for the discovery of superfluid phases in liquid helium-three, have spurred even greater interest [3] in this standard textbook example of a phase transition.

In this paper we consider an ideal quantum gas of bosons which are either *permanent* (i.e. number-conserving as, e.g., ^{4}He atoms) or *ephemeral* [4] (i.e. *non*-number-conserving as, e.g., photons), each possessing an excitation energy as a function of the wavenumber k, i.e. the bosonic 'dispersion relation'

$$\varepsilon_k = c_s k^s \qquad \text{with } s > 0 \tag{1}$$

in $d > 0$ dimensions. For ordinary (non-relativistic) bosons of mass m *in vacuo* with *quadratic* dispersion relation, $s = 2$ and $c_s = \hbar^2/2m$. There exists a non-zero absolute temperature T_c below which a macroscopic occupation emerges for *one* quantum state (of infinitely many), only if $d > 2$ [5]. (The $d = 2$ case, in fact, displays the *same* [6] smooth, singularity-free, temperature-dependent specific heat for either bosons or fermions). The Bose–Einstein (BE) distribution function $n_k \equiv [e^{\beta[\varepsilon_k - \mu(T)]} - 1]^{-1}$ is by definition the average number of bosons in a given state ε_k. When summed over all states it yields the total number of bosons N, each of mass m, of which, say $N_0(T)$ are in the lowest state ε_k ($\to 0$ as one takes the thermodynamic limit). Explicitly, at any given absolute temperature T,

$$N = N_0(T) + \sum_{k\neq 0} n_k \equiv N_0(T) + \sum_{k\neq 0} \frac{1}{e^{\beta[\varepsilon_k - \mu(T)]} - 1} \qquad (2)$$

where $\beta \equiv 1/k_B T$ and $\mu(T) \leqslant 0$ is the chemical potential. The latter inequality ensures a non-negative summand, as by definition it must be. Einstein surmised that for $T > T_c$, $N_0(T)$ is negligible compared with N; while for $T < T_c$, $N_0(T)$ is a sizeable fraction of N. At precisely $T = T_c$, $N_0(T_c) \simeq 0$ *and* $\mu \simeq 0$, while at $T = 0$ the last term in (2) vanishes so that $N = N_0(0)$ (namely, the absence of any exclusion principle). Note that $\mu = 0^-$ for *all* T such that $0 < T < T_c$ since from (2) $N_0(T) = (e^{-\beta\mu} - 1)^{-1}$ implies that $e^{\beta\mu} = N_0(T)/[N_0(T) + 1] < 1$, and this quantity approaches 1^- over this *entire* temperature range since $N_0(T)$ on cooling grows to a sizeable fraction of N which in turn is macroscopic.

2. Transition temperature

Since $N_0(T)$, the number of bosons in the lowest energy state (with $k = 0$), just ceases to be negligible (compared with N) at and below T_c, then $N_0(T_c)/N_0(0) = 0$ leads straightforwardly, after some algebra, from (2) to the *general T_c-formula*

$$T_c = \frac{c_s}{k_B}\left[\frac{s\,\Gamma(d/2)\,(2\pi)^d\, n}{2\pi^{d/2}\,\Gamma(d/s)\, g_{d/s}(1)}\right]^{s/d} \propto n^{s/d} \qquad (3)$$

where $g_{d/s}(1)$ are certain dimensionless numbers (see the appendix), $\Gamma(\sigma)$ is the familiar gamma function and $n \equiv N/L^d$ the d-dimensional boson number-density. Also using (3), the condensate fraction then simplifies to

$$\frac{N_0(T)}{N_0(0)} = 1 - (T/T_c)^{d/s} \qquad T \leqslant T_c \qquad (4)$$

which is 1 at $T = 0$ and 0 for $T \geqslant T_c$. The reason for these simple, closed-expression results are the so-called *Bose functions* $g_\sigma(z)$ (see the appendix) to which the summation in (2) reduces. A somewhat different derivation of a similar, though not identical, result is found in the PC-oriented textbook [8].

These formulae are valid for all $d > 0$ and $s > 0$. For $s = 2$, $c_s = \hbar^2/2m$ and $d = 3$ dimensions, equations (3) and (4) become

$$T_c = \frac{2\pi\hbar^2 n^{2/3}}{mk_B[\zeta(3/2)]^{2/3}} \simeq \frac{3.31\hbar^2 n^{2/3}}{mk_B} \quad \text{and} \quad \frac{N_0(T)}{N_0(0)} = 1 - (T/T_c)^{3/2} \qquad (5)$$

since $\zeta(3/2) \simeq 2.612$. These are the familiar results for the 'ordinary' BEC in 3D observed recently [1]. Note also that for $0 < d \leqslant s$, $T_c = 0$, since (A2) diverges for $d/s \leqslant 1$. This behaviour of (A2) implies that BEC does *not* occur for s-dispersion-relation bosons for $d \leqslant s$ dimensions, which is consistent with the well known fact that BEC does *not* occur for free space, quadratic-dispersion-relation (i.e. non-relativistic) bosons for dimensions equal to or smaller than two. However, for $s = 1$ BEC *can* occur for all $d > 1$. In fact a *linear* dispersion relation holds ([9, p 33], [10]) for a Cooper pair of electrons moving not in a vacuum but in the Fermi sea. Such pairs can thus Bose–Einstein condense [11], fortuitously, in *all* dimensions where actual superconductors have been found to exist, down to the quasi-one-dimensional organics [12] consisting of parallel chains of molecules. Although the creation/annihilation operators of Cooper pairs do *not* obey the usual Bose commutation rules [9, p 38], they *do satisfy BE statistics* [11] since an indefinitely large number of pairs, each with fixed momenta $\hbar\boldsymbol{k}_1$ and $\hbar\boldsymbol{k}_2$, correspond to different relative momenta $\hbar\boldsymbol{k} \equiv \hbar(\boldsymbol{k}_1 - \boldsymbol{k}_2)/2$ but add vectorially to the *same* total (centre-of-mass) momentum $\hbar\boldsymbol{K} \equiv \hbar(\boldsymbol{k}_1 + \boldsymbol{k}_2)$. Antiferromagnetic *magnons* also have $s = 1$, while ferromagnetic ones correspond to $s = 2$ [13, pp 458, 468], but neither can BE condense as their number at any given T is indefinite.

3. Internal energy

The internal energy $U(L^d, T)$ of an ideal many-boson system, where each boson has excitation energy ε_k, can be written as

$$U(L^d, T) = \sum_k \varepsilon_k n_k \equiv \sum_k \frac{\varepsilon_k}{e^{\beta(\varepsilon_k - \mu)} - 1} \tag{6}$$

and eventually leads to a general expression valid for *all temperatures*

$$\frac{U(L^d, T)}{Nk_BT} = \frac{d}{s} \frac{g_{d/s+1}(z)}{g_{d/s}(1)} t^{d/s} \tag{7}$$

where $t \equiv T/T_c$. For $T > T_c$, $N_0(T) = 0$, so using (3) we obtain the remarkably simple relation

$$g_{d/s}(z) = \frac{g_{d/s}(1)}{t^{d/s}} \qquad t \geqslant 1. \tag{8}$$

Thanks to (8), equation (7) simplifies for $T \geqslant T_c$ to

$$\frac{U(L^d, T)}{Nk_BT} = \frac{d}{s} \frac{g_{d/s+1}(z)}{g_{d/s}(z)} \xrightarrow{T\to\infty} d/s \qquad t \geqslant 1 \tag{9}$$

where the limiting result follows from the fact (see equation (A2) below) that $g_\sigma(z) \xrightarrow{T\to\infty} z$, if $\sigma > 1$. Equation (9) is a generalization of the 'classical partition theorem', more commonly recalled for $d = 3$ and $s = 2$.

For $T \leqslant T_c$, or $t \leqslant 1$, $z = 1$, so equation (7) becomes

$$\frac{U(L^d, T)}{Nk_BT} = \frac{d}{s} \frac{g_{d/s+1}(1)}{g_{d/s}(1)} t^{d/s} \propto T^{d/s}. \tag{10}$$

If $d = 3$ and $s = 1$ as in a photon gas, this is just the 'Stefan–Boltzmann law' $U(T)/L^d = \sigma T^4$ of 'black-body' radiation, with σ a constant. In this case, however, $T_c = \infty$ since $\mu = 0$ *for all* T, as a consequence of the *indefiniteness* in the total number of particles.

Figure 1 shows the internal energy (in units of Nk_BT) as a function of temperature (in units of T_c as given by (3)) for $(d, s) = (3, 2)$, $(2, 1)$ and $(3, 1)$. Only the last case possesses a slope discontinuity precisely at T_c, while the first two cases merely change in curvature as T increases, namely, from 'concave up' to 'concave down.' The asymptotes at $U/Nk_BT = \frac{3}{2}$, 2 and 3 are just the respective classical (high-temperature) limits (9).

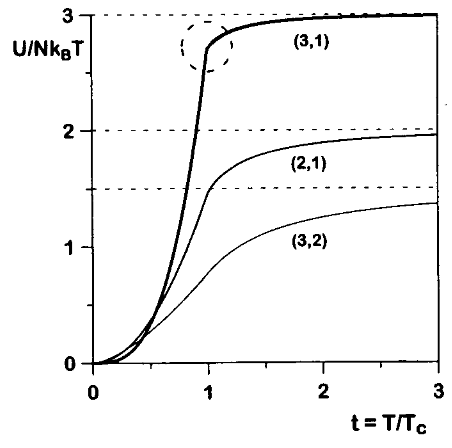

Figure 1. Internal energy U as a function of $t = T/T_c$ for $d/s = 3/2$, $2/1$ and $3/1$. Only the latter case exhibits a slope discontinuity (dashed circle).

The pressure can also be determined for any d and s, though we omit details, and leads to a generalization of the familiar relation $PV = \frac{2}{3}U$ for an ideal gas of either bosons or fermions in the non-relativistic limit and confined within a volume V, namely

$$PL^d = \frac{s}{d}U \tag{11}$$

which is cited in [7, p 190].

4. Specific heat

The constant-volume specific heat C_V *for all* T is defined by $C_V = (\partial U/\partial T)_{N,V}$. For $T < T_c$, $\mu = 0^-$ and $z = 1^-$, and equation (10) leads to

$$C_V(T) = Nk_B \frac{(d/s)(d/s+1)g_{d/s+1}(1)}{g_{d/s}(1)} t^{d/s} \propto T^{d/s}. \tag{12}$$

In three dimensions, Debye acoustic phonons ($s = 1$) correspond to $d/s = 3$ and hence the familiar T^3 behaviour; Bloch (ferromagnetic) magnons ($s = 2$) to $d/s = \frac{3}{2}$, [13, pp 124, 482], and thus the well known $T^{3/2}$ law. However, for $T > T_c$ a result very different from (12) emerges. After some simple algebra, the specific heat jump (if any) at T_c will be

$$[\Delta C_V/Nk_B]_{T_c} \equiv [C_V(T_c^-) - C_V(T_c^+)]/Nk_B = \frac{(d/s)^2 g_{d/s}(1)}{g_{d/s-1}(1)}. \tag{13}$$

Because $g_\sigma(1) = \infty$ for $\sigma \leqslant 1$ (see the appendix) there is *no jump discontinuity in the specific heat for all* $d/s \leqslant 2$. The commonest instance of this is the 3D ideal Bose gas (with $s = 2$) exhibiting merely a cusp in its temperature-dependent specific heat at T_c, i.e. a discontinuity only in the slope but not in the value of $C_V(T)$. Also, since $g_\sigma(1) \equiv \zeta(\sigma)$ if $\sigma > 1$ (see the appendix), for $d/s > 1$ one has the quantity (to be discussed further)

$$\frac{\Delta C_V(T_c)}{C_V(T_c^-)} = \frac{(d/s)\zeta^2(d/s)}{(d/s+1)\zeta(d/s-1)\zeta(d/s+1)}. \tag{14}$$

At high temperatures (i.e. the classical regime) occupation in any given state $\boldsymbol{k}$ is expected to be minute, so from equations (1) and (2) with each summand very small

$$N \xrightarrow{T\to\infty} e^{\beta\mu} \sum_{\boldsymbol{k}} e^{-\beta C_s k^s} \tag{15}$$

ultimately allows one to write

$$C_V/Nk_B \xrightarrow{T\to\infty} d/s. \tag{16}$$

This is the *generalized Dulong–Petit law*. Recalling that $C_V = (\partial U/\partial T)_{N,V}$ this checks with (9).

Figure 2 depicts the constant-volume specific heat C_V (in units of Nk_B) versus $t \equiv T/T_c$. Only for $(d, s) = (3, 1)$ is there a jump discontinuity, while for (2, 1) and (3, 2) the singularity is merely a 'cusp', all in keeping with the properties of the internal energy already mentioned in connection with figure 1. Figure 3 illustrates how the specific-heat jump discontinuity vanishes for all $d/s \leqslant 2$, as evident from (13), and how it rises for $d/s > 2$. Remarkably, the BCS value of 0.588 (marked on the figure) associated [15] with an ideal gas of *fermionic* excitations (called 'bogolons' or 'bogoliubons') is only slightly smaller than the value 0.609 marked by the dashed lines and which corresponds [11] to an ideal gas of *bosonic* Cooper pairs with $s = 1$ in three dimensions. A bogolon 'quasiparticle' [16] is a linear combination of a fermion particle and a fermion 'hole'.

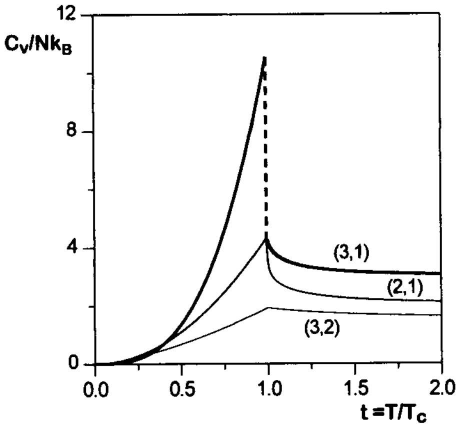

Figure 2. Constant-volume specific heat C_V as a function of $t = T/T_c$ for $d/s = 3/2$, $2/1$, and $3/1$. Only the latter case exhibits a jump discontinuity (dashed vertical line).

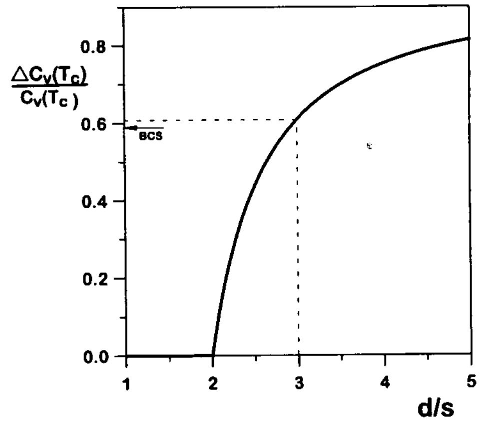

Figure 3. Magnitude of jump discontinuity in the specific heat as a function of d/s, the 3D *bosonic* value of 0.609 [11] being just above the BCS value of 0.588 [15] corresponding to *fermionic* excitations.

5. Conclusions

We have presented a didactic discussion appropriate for university-level physics of the closed, analytical forms assumed by several thermodynamic functions of an ideal gas of N bosons in a 'volume' L^d, in $d > 0$ dimensions, for bosons each of energy $\varepsilon_k = c_s k^s$, with $s > 0$, where c_s is a constant and k the boson wavenumber. Bose–Einstein condensation occurs (i.e. with a non-zero transition temperature T_c) *only if* $d/s > 1$. Moreover, if $d/s > 1$, $T_c \propto n^{s/d}$, where $n \equiv N/L^d$, and the 'condensate fraction' $N_0/N = 1 - (T/T_c)^{d/s}$, where N_0 is the number of bosons in the lowest ($k = 0$) single-boson quantum state. The system internal energy $U = (d/s)PL^d$, where P is the thermodynamic pressure, and for $T < T_c$, $U \propto T^{d/s+1}$. The constant-volume specific heat has a jump discontinuity at T_c *only if* $d/s > 2$. Finally, at high temperatures the expected classical limits, such as 'equipartition' and the Dulong–Petit law, are recovered.

Note added in proof. After this paper was completed, we learned that some of the results reported here previously appeared in [17].

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Appendix. A word about Bose integrals

The volume $V_d(R)$ of a hypersphere of radius R in $d \geqslant 0$ dimensions is found to be $V_d(R) = \pi^{d/2}R^d/\Gamma(1 + d/2)$ [7, p 504]. For $d = 3$ this is just $4\pi R^3/3$; for $d = 2$ it is the area πR^2 of a circle of radius R; for $d = 1$ it is the 'diameter' $2R$ of a line of 'radius' R; and for $d = 0$ it is unity. Using this for $d > 0$, and since the allowed states of a particle in a 'box' with 'sides' L correspond to the sites in k-space of a simple-cubic lattice with lattice spacing $2\pi/L$, the summation in (2) over the d-dimensional vector $\boldsymbol{k}$ becomes an integral over *positive* $k \equiv |\boldsymbol{k}|$, which in the thermodynamic limit (where $2\pi/L$ becomes infinitesimally small) is simply

$$\sum_{k\neq 0} \longrightarrow \frac{2\pi^{d/2}}{\Gamma(d/2)}\left(\frac{L}{2\pi}\right)^d \int_{0^+}^{\infty} \mathrm{d}k\, k^{d-1} \tag{A1}$$

with the first prefactor reducing as it should to 2, 2π and 4π for $d = 1$, 2 and 3, respectively. The sum in (2) is then an elementary integral expressed in terms of the so-called *Bose integrals* [7, pp 159, 506]:

$$g_\sigma(z) \equiv \frac{1}{\Gamma(\sigma)}\int_0^\infty \mathrm{d}x\, \frac{x^{\sigma-1}}{z^{-1}\mathrm{e}^x - 1} = \sum_{l=1}^{\infty} \frac{z^l}{l^\sigma} \tag{A2}$$

where $z \equiv \mathrm{e}^{\mu/k_BT}$ is known as the *'fugacity'*. For $z = 1$ and $\sigma \geqslant 1$ equation (A2) coincides with the Riemann zeta-function $\zeta(\sigma)$, which converges for $\sigma > 1$ and diverges for $\sigma = 1$ when it becomes the celebrated harmonic series $g_1(1) \equiv \zeta(1) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots$. For $z = 1$ and $0 < \sigma < 1$ the series (A2) clearly diverges even more severely than $\zeta(1)$.

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