

# Bose-Einstein Condensation and Condensate Tunneling

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We consider Bose-Einstein condensation in a small cube and describe effects induced by the confinement. We also sketch an analogue of the Josephson effect for neutral particles, which can be realized when two almost degenerate states in a double well potential are occupied by a macroscopic number of Bosons.

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At very low temperatures, a major fraction of the particles of an ideal Bose gas accumulates in the quantum mechanical ground state. This effect, discussed by Einstein [1] already in 1924, has resisted its experimental verification for seventy years. However, after recent advances in cooling and trapping of neutral atoms [2–5], the realization of Bose-Einstein condensation in small traps appears to be only a matter of time now. When a Bose gas consists of some  $10^7$  to  $10^8$  particles confined to a small volume, the physical boundary conditions for the wave functions influence its properties in a measurable way. The condensation temperature is shifted upwards, the temperature dependence of the heat capacity is modified, and the quantum mechanical zero point pressure becomes non-negligible. An intriguing question emerges if the confining potential has the shape of a double well: Could there be coherent quantum tunneling of the entire condensate?

An ideal Bose gas, consisting of  $N$  noninteracting particles of mass  $m$  moving freely in a large volume  $V$ , is known to “condense” in the ground state [6–9] if the temperature  $T$  is lower than

$$T_0 = \frac{2\pi\hbar^2}{m\kappa} \left( \frac{N}{2.612V} \right)^{2/3}. \quad (1)$$

Here  $\hbar$  and  $\kappa$  are Planck’s and Boltzmann’s constants, respectively. When F. London [6] derived this formula in 1938, he used periodic boundary conditions for the quantum mechanical wave functions  $\psi$ . Working with a cube-sized volume of side length  $L$ , i.e.,  $V=L^3$ , he

stipulated that  $\psi$  should take on equal values at opposite points on the surface of the cube. The use of these mathematically convenient, but physically artificial boundary conditions can be justified as long as the de Broglie wavelength of the Bose particles at temperature  $T$ , i.e., the thermal wavelength

$$\lambda_T = \hbar \sqrt{\frac{2\pi}{m\kappa T}}, \quad (2)$$

is negligibly small compared to the linear extension  $L$  of the system. If that is not the case, either because  $T$  is too low or because  $L$  itself is small, then the confinement has measurable effects on the properties of the Bose gas. A thorough understanding of these effects will be of practical importance when Bose-Einstein condensation can be realized in micro-sized cavities.

To estimate effects caused by the confinement, physically correct boundary conditions must be used, i.e., the wave functions must be zero at the surface of a cube with impenetrable walls. In this case the number of accessible quantum states is lower than it would be for a hypothetical system of equal volume, but with periodic wave functions. The temperature for the onset of Bose-Einstein condensation then is no longer given by (1), but rather by

$$T_c = T_0 \left[ 1 - 0.7656 \frac{\lambda_{T_0}}{L} \ln \left( 1.535 \frac{\lambda_{T_0}}{L} \right) \right]. \quad (3)$$

The parameter that determines the shift of the condensation temperature,  $\lambda_{T_0}/L$ , is the ratio of the thermal wavelength at  $T_0$  and the system size. This ratio is generally small, since  $\lambda_{T_0} = 1.377 L/N^{1/3}$  measures the mean particle distance. The true condensation temperature  $T_c$  is higher than  $T_0$ . This is a consequence of the missing states (as compared to the hypothetical

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periodic system): because there are fewer states available, the large-scale occupation of the ground state has to start already at higher temperatures.

Remarkably,  $\lambda_{T_0}/L$  can be expressed solely in terms of the total number of particles:  $\lambda_{T_0}/L = 1.377 N^{-1/3}$ . If the particle number  $N$  is reduced, while the volume  $V$  remains the same, then the absolute value of the condensation temperature decreases according to (1), but the relative magnitude of the finite size corrections in (3) increases. Figure 1 shows the relative shift of condensation temperature,  $(T_c - T_0)/T_0$ , as a function of the particle number  $N$ .

An interesting and somewhat counterintuitive property of the ideal Bose gas below  $T_c$  is the independence of its heat capacity  $C_V$  of the number of particles. This property is preserved if the gas is confined to a cube with impenetrable walls:

$$C_V = 5.031 \kappa \left( \frac{L}{\lambda_T} \right)^3 \left[ 1 - 0.981 \frac{\lambda_T}{L} + 0.918 \left( \frac{\lambda_T}{L} \right)^2 \right]. \quad (4)$$

The first factor on the right hand side is the famous result for periodic boundary conditions, according to which  $C_V$  should be proportional to  $T^{3/2}$ . But this behaviour is modified by the confinement. In the brackets are shown the resulting corrections for the relative size  $\lambda_T/L$  and  $(\lambda_T/L)^2$ . This formula is valid for values of  $\lambda_T/L$  between  $1.377 N^{-1/3}$  and about 0.3. At even lower temperatures,  $C_V$  decreases exponentially. An example for the magnitude of the corrections is shown in Figure 2.

For temperatures below  $T_c$ , the pressure  $P$  exerted by the confined Bosons is

$$P = 1.341 \frac{\kappa T}{\lambda_T^3} \left[ 1 - 1.226 \frac{\lambda_T}{L} + 1.529 \left( \frac{\lambda_T}{L} \right)^2 \right] + \frac{2}{3} \frac{N \varepsilon_0}{V}. \quad (5)$$

There are not only corrections with a relative size of powers of  $\lambda_T/L$  to the pressure in a periodic system, but also the zero point pressure  $P_0 = 2N\varepsilon_0/(3V)$  appears. It is a basic statement of quantum mechanics that particles restricted to move in a finite region must have a positive ground state energy  $\varepsilon_0$ . This ground state energy is responsible for the zero point pressure, which would be the total pressure of the condensate at  $T=0$ . In the case of periodic boundary conditions, the wave functions could be continued to periodic functions defined in all of space. Hence the ground state energy would be equal to zero for these artificial

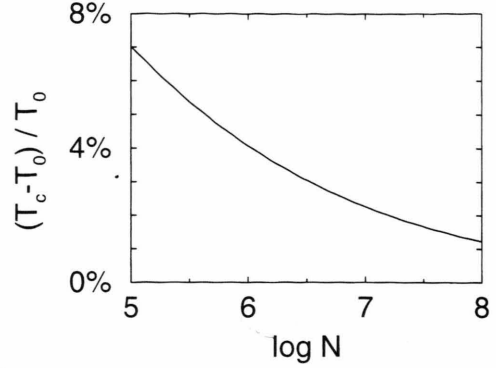


Fig. 1. Shift of the condensation temperature  $T_c$  of an ideal Bose gas in a cube with impenetrable walls, relative to the condensation temperature  $T_0$  for a hypothetical system with periodic boundary conditions. This relative shift depends only on the total number of particles,  $N$ .

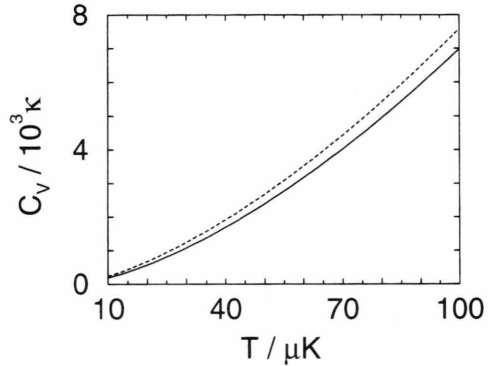


Fig. 2. Heat capacity  $C_V$  of an ideal Bose gas below  $T_c$ , confined to a cube of side length  $L = 1 \mu\text{m}$ . The particle mass is that of  $^4\text{He}$ ,  $m = 6.65 \cdot 10^{-27} \text{ kg}$ . The broken line shows the heat capacity for the hypothetical periodic system; the solid line is the actual heat capacity according to (4). Because of the reduced number of available states the actual heat capacity is smaller than that for periodic boundary conditions. Both heat capacities are independent of the number of particles,  $N$ . The graphs are valid as long as the temperature of the gas is lower than the condensation temperature, which does depend on  $N$ . For example,  $T_c = 1.9 \cdot 10^4 \mu\text{K}$  for  $10^7$  particles.

boundary conditions, and there were no zero point pressure. However, Fig. 3 demonstrates that in micro-sized cavities  $P_0$  can give a substantial contribution to the total pressure, even at moderately low temperatures.

Since  $T_0$  is proportional to  $1/m$ , lighter particles undergo Bose-Einstein condensation already at higher temperatures. In fact, indications for Bose-Einstein condensation of excitons have already been ob-

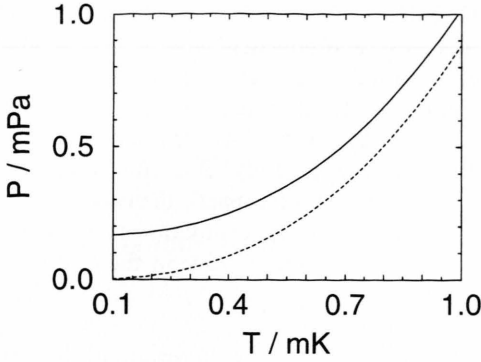


Fig. 3. Pressure  $P$  exerted by a sample of  $10^7$  ideal Bose particles in a cube with side length  $L=1\text{ }\mu\text{m}$ . The mass of the particles is again that of  $^4\text{He}$ . The broken line denotes the pressure in a hypothetical periodic system. The solid line is the actual pressure according to (5). The contribution of the zero point pressure is  $P_0=0.165\text{ mPa}$ . The condensation temperature is  $T_c=19.05\text{ mK}$ , shifted upwards from  $T_0$  by 2.3%.

served [10], and even the possibility for the condensation of Positronium gas has been discussed recently [11]. Ultracold atoms in traps [2–5], although heavier, appear to offer particularly exciting possibilities not only for realizing Bose-Einstein condensation, but also for performing well-controlled experiments with the condensate. Trapping is achieved by inhomogeneous electromagnetic fields which lead to a dependency of the atomic energy levels on the position in the trap. The atoms in a trap do therefore not move freely but feel the influence of the trapping potential. This potential is not that of a box with impenetrable walls, but varies smoothly in space and can be approximated by the potential of a harmonic oscillator [3]. This has decisive consequences for Bose-Einstein condensation. For Bosons in an isotropic harmonic oscillator potential the condensation temperature becomes

$$T_c = \frac{\hbar\omega}{\kappa} \left( \frac{N}{1.202} \right)^{1/3}. \quad (6)$$

The estimate  $\omega \approx 100\text{ s}^{-1}$  for the oscillator frequency, which appears to be quite realistic, gives  $T_c \approx 0.15\text{ }\mu\text{K}$  for  $N=10^7$  trapped particles. For Cesium atoms, the extension of the ground state wave function would be about  $10\text{ }\mu\text{m}$ . The heat capacity for such a system is quite different from that of free Bosons, namely, proportional to  $T^3$ :  $C_V = \kappa(2\pi^4/15) \cdot (\kappa T/\hbar\omega)^3$  below  $T_c$ .

Now suppose that a large number of atoms has been successfully cooled down and that the condensate is trapped in the neighborhood of the potential

minimum. Next, suppose that the electromagnetic fields generating the trapping potential are instantaneously modified such that a second minimum appears, equally shaped as the one initially occupied by the condensate. The new potential then is a symmetric double well, and the condensate will start to tunnel into the new minimum. The tunneling time is determined by the ground state splitting  $\Delta E$ , i.e., by the difference of the two lowest energy eigenvalues of the symmetric double well system. Assuming  $\Delta E = \hbar\omega/100$ , one finds a tunneling time of the order of seconds – quite within the range of achievable trapping times. Since imaging techniques allow to record the positions of the atoms in a trap (albeit in a destructive manner), a fascinating possibility emerges: it might become feasible to directly observe a tunneling Bose condensate in a double well potential!

A closer look at this scenario reveals an even more spectacular phenomenon. The single particle spectrum of the double well is a series of doublets, each one consisting of two closely spaced energy levels that are separated by larger energy gaps from the adjacent doublets. At  $T=0$  all particles would be condensed in the state of lowest energy, i.e., in the lower member of the ground state doublet. This state has a symmetric wave function. Hence, at each moment the numbers of particles in the two wells would be identical. At non-zero temperatures, however, when  $\kappa T$  is larger than the ground state splitting  $\Delta E$ , both members of the ground state doublet can be populated almost equally. If, moreover,  $\kappa T$  remains small compared to the energy gap that separates the ground state doublet from the first excited doublet, the occupation numbers of the other states are still negligibly small. Then two states are occupied by a macroscopic number of particles, and the total wave function of the system is a coherent superposition of the wave functions of its two components.

Now one can introduce two complex amplitudes  $a_1(t)$  and  $a_2(t)$  such that  $|a_1(t)|^2$  and  $|a_2(t)|^2$  describe the number of particles that can be found at time  $t$  in the first and second well, respectively. The Schrödinger equation for the two-component system is

$$\begin{aligned} i\hbar \frac{da_1(t)}{dt} &= \frac{\Delta E}{2} a_2(t), \\ i\hbar \frac{da_2(t)}{dt} &= \frac{\Delta E}{2} a_1(t). \end{aligned} \quad (7)$$

If all  $N$  particles occupy the first well at  $t=0$ , its solution reads  $a_1(t) = i\sqrt{N} \cos(\Delta E t/2\hbar)$ , and  $a_2(t) = \sqrt{N}$

$\sin(\Delta E t/2\hbar)$ , i.e.,  $a_1$  and  $a_2$  oscillate in time. Does that mean that there can be a macroscopic, oscillating current of particles between the two wells, even without any external drive? Yes, it does.

The situation considered here is reminiscent of a Josephson junction, where Cooper pairs tunnel through a thin insulating layer that separates two superconductors [12, 13]. But there is a crucial difference. The Cooper pairs in a Josephson junction carry electrical charge. Therefore, both sides of the junction have to be connected to a battery in order to prevent either side from being charged up and to keep their potentials constant. In the present case of a Bose condensate in a double well the particles are electrically neutral, so that no charging can occur which would counteract tunneling.

Both wave functions of the two components of the Bose condensate, each one describing a macroscopic number of particles, extend over both wells. The key point that allows coherent, oscillating tunneling of the

whole condensate is the fact that the relative phase between the two components,  $\phi(t) = \phi_0 + (\Delta E/\hbar)t$ , grows linearly with time. Initially the two waves interfere constructively in the first well and destructively in the second, so that the probability for finding all particles in the first well is unity. But after the time  $\tau = \hbar\pi/\Delta E$  the relative phase between the two components has grown by  $\pi$ , and the situation is reversed: now there is destructive interference in the first well and constructive in the second; the condensate has tunneled to the second well.

This curious effect of coherent tunneling of the entire Bose condensate, or of constructive and destructive interference of two wave functions that describe a macroscopic number of particles, is another striking manifestation of quantum mechanics on a large scale. Once Bose-Einstein condensation in atom traps has been achieved, it will certainly be exciting to hunt for the experimental confirmation of condensate oscillations.

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