Bose-Einstein condensation
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A **Bose–Einstein condensate (BEC)** is a state of matter of a dilute gas of weakly interacting bosons confined in an external potential and cooled to temperatures very near absolute zero (0 K). Under such conditions, a large fraction of the bosons occupy the lowest quantum state of the external potential, at which point quantum effects become apparent on a macroscopic scale. This state of matter was first predicted by Satyendra Nath Bose and Albert Einstein in 1924–25. Bose first sent a paper to Einstein on the quantum statistics of light quanta (now called photons). Einstein was impressed, translated the paper himself from English to German and submitted it for Bose to the *Zeitschrift für Physik*, which published it. Einstein then extended Bose's ideas to material particles (or matter) in two other papers.

Seventy years later, the first gaseous condensate was produced by Eric Cornell and Carl Wieman in 1995 at the University of Colorado at Boulder NIST-JILA lab, using a gas of rubidium atoms cooled to 170 nK. For their achievements Cornell, Wieman, and Wolfgang Ketterle at MIT received the 2001 Nobel Prize in Physics. In November 2010 the first photon BEC was observed.

The slowing of atoms by the use of cooling apparatus produced a singular quantum state known as a **Bose condensate** or **Bose–Einstein condensate**. This phenomenon was predicted in 1925 by generalizing Satyendra Nath Bose's work on the statistical mechanics of (massless) photons to (massive) atoms. (The Einstein manuscript, once believed to be lost, was found in a library at Leiden University in 2005.) The result of the efforts of Bose and Einstein is the concept of a Bose gas, governed by Bose–Einstein statistics, which describes the statistical distribution of identical particles with integer spin, now known as bosons. Bosonic particles, which include the photon as well as atoms such as helium-4, are allowed to share quantum states with each other. Einstein demonstrated that cooling bosonic atoms to a very low temperature would cause them to fall (or "condense") into the lowest accessible quantum state, resulting in a new form of matter.

http://en.wikipedia.org/wiki/Bose%E2%80%93Einstein_condensate

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1. Bose-Einstein distribution function

The Bose-Einstein distribution function is defined as

$$f(\varepsilon,T)=\frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$

where $\beta=\dfrac{1}{k_BT}$ and k_B is the Boltzmann constant. The occupancy of the ground state at $\varepsilon=0$ is

$$N_0(T) = f(\varepsilon = 0, T) = \frac{1}{e^{-\beta\mu} - 1}$$

The total number of particles *N* should be given by

$$N = \lim_{T\to 0} \frac{1}{e^{-\beta\mu} - 1} \approx \lim_{T\to 0} \frac{1}{1 - \beta\mu - 1} \approx -\frac{k_B T}{\mu}$$

For very low temperatures, the chemical potential μ is very close to zero and should be negative.

$$\mu = -\frac{k_B T}{N} < 0$$

The chemical potential in a boson system must always be lower in energy than the ground state.

Suppose that all the bosons are in the single-particle state of the lowest energy ε_1. The total energy is then

$$U_G = N\varepsilon_1$$

Since the ground state is not degenerate

$$N = \lim_{T\to 0} \frac{1}{e^{\beta(\varepsilon_1 - \mu)} - 1} = \lim_{T\to 0} \frac{1}{1 + \beta(\varepsilon_1 - \mu) - 1} = \frac{k_B T}{\varepsilon_1 - \mu}$$

if $\mu < \varepsilon_1$ (in this case $e^{\beta(\varepsilon_1 - \mu)}$>1 and is very close to 1). This equation yields to

$$\mu = \varepsilon_1 - \frac{k_B T}{N}$$

((**Example**))

For $N = 10^{22}$ and $T = 1$ K, $\mu = -1.4 \times 10^{-38}$ erg <0.

2. Occupancy of the ground state

Density of states for a particle of spin zero is given by

$$D(\varepsilon) = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} \qquad (g = 1)$$

where the energy vs k is given by

$$\varepsilon = \frac{\hbar^2 k^2}{2m}$$

The number N (fixed) is expressed by

$$N = N_e(T,z) + N_0(T) = \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon + N_0(T)$$

where z is the fugacity (which will be defined later), $N_e(T)$ is the number of atoms in excited states (the number of atoms in the normal phase) and $N_0(T) = f(\varepsilon = 0, T)$ is the number of atoms in the ground state (number of atoms in the condensed phase)

Here we note that we must be cautious in substituting

$$D(\varepsilon) = \frac{gV}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}$$

into

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon$$

At high temperature there is no problem. But at low temperatures there may be a pile-up of particles in the ground state $\varepsilon = 0$; then we will get an incorrect result for N. This is because $D(\varepsilon) = 0$ in the approximation we are using, whereas there is actually one state at $\varepsilon = 0$. If this one state is going to be important, we should write

$$\widetilde{D}(\varepsilon) = \delta(\varepsilon) + D(\varepsilon)$$

with $g = 1$, where $\delta(\varepsilon)$ is the Dirac delta function.

$$N = \int_0^\infty \widetilde{D}(\varepsilon) f(\varepsilon) d\varepsilon = \int_0^\infty [\delta(\varepsilon) + D(\varepsilon)] f(\varepsilon) d\varepsilon = N_0(T) + N_e(T,z)$$

Here we have

$$N_0(T) = \frac{1}{e^{-\beta\mu} - 1} = \frac{1}{\frac{1}{z} - 1}$$

and

$$N_e(T, z) = \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\sqrt{\varepsilon}}{\frac{1}{z} e^{\beta\varepsilon} - 1} d\varepsilon$$

where

$z = e^{\beta\mu}$.

With $x = \beta\varepsilon$, $N_e(T, z)$ can be rewritten as

$$\begin{aligned}
N_e(T, z) &= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty k_B T dx \frac{(k_B T)^{1/2}\sqrt{x}}{\frac{1}{z} e^x - 1} \\
&= \frac{V}{4\pi^2}(4\pi)^{3/2}\left(\frac{m k_B T}{2\pi\hbar^2}\right)^{3/2} \int_0^\infty dx \frac{\sqrt{x}}{\frac{1}{z} e^x - 1} \\
&= V n_Q \frac{2}{\sqrt{\pi}} \int_0^\infty dx \frac{\sqrt{x}}{\frac{1}{z} e^x - 1} \\
&= V n_Q \varsigma_{3/2}(z)
\end{aligned}$$

Note that the integral (for z<1) is obtained as

$$\varsigma_{3/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty dx \frac{\sqrt{x}}{\frac{1}{z} e^x - 1} = \frac{2}{\sqrt{\pi}} \int_0^\infty dx \frac{z e^{-x}\sqrt{x}}{1 - z e^{-x}},$$

$$\begin{aligned}\varsigma_{3/2}(z=1) &= \frac{2}{\sqrt{\pi}}\int_0^\infty dx\frac{\sqrt{x}}{e^x-1}\\ &= \frac{2}{\sqrt{\pi}}\Gamma(\frac{3}{2})\varsigma(\frac{3}{2})\\ &= \frac{2}{\sqrt{\pi}}\frac{\sqrt{\pi}}{2}\times 2.61238\\ &= 2.61238\end{aligned}$$

where $\varsigma_{3/2}(z)$ is described by

$$\varsigma_{3/2}(z) \to \text{PolyLog}[\frac{3}{2}, z]$$

in Mathematica. Then we get

$$N_e(T,z) = Vn_Q(T)\varsigma_{3/2}(z)$$

where $\varsigma_{3/2}(z)$ is the zeta function and $\varsigma_{3/2}(z=1) = 2.61238$, and $n_Q(T)$ is defined as

$$n_Q(T) = (\frac{mk_BT}{2\pi\hbar^2})^{3/2}$$

which is called the quantum concentration. It is the concentration associated with one atom in a cube equal to the thermal average de Broglie wavelength λ_{th}. The de Broglie wavelength is given by

$$n_Q(T) = \frac{1}{\lambda_{th}^3}$$

where

$$\lambda_{th} \approx \frac{\hbar}{m\langle v\rangle}$$

and $\langle v\rangle$ is the average thermal velocity.

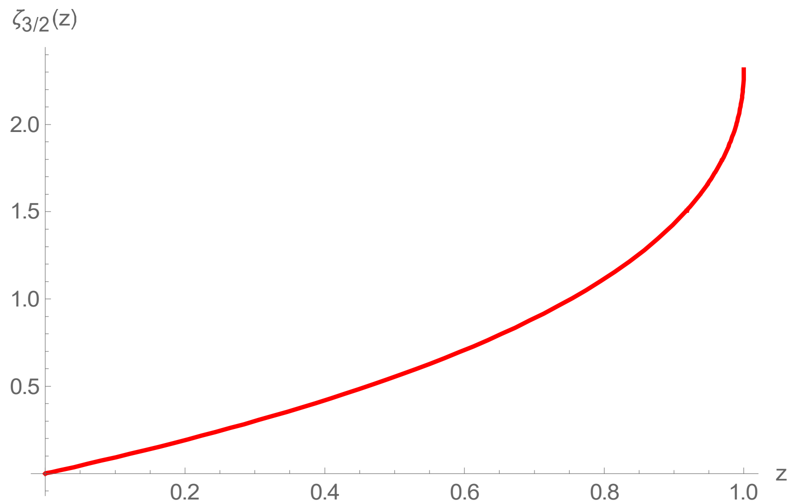

Fig. Plot of $\varsigma_{3/2}(z)$ as a function of z. $\varsigma_{3/2}(z=1) = 2.61238$

3. Bose-Einstein-Condensation temperature T_E

We start our discussion with the equation given by

$$N = N_e(T, z) + N_0(T)$$

We note that $N_e(T, z=1)$ has a maximum value when $z = 1$. Since N is constant, N should be larger than this maximum of $N_e(T, z=1)$ at $z = 1$.

$$N \geq N_e(T, z=1) = V n_Q(T) \varsigma_{3/2}(z=1) .$$

Here we define the temperature T_E (the Einstein temperature for Bose-Einstein condensation) at which

$$N = N_e(T_E, z=1) .$$

or

$$N = V n_Q(T_E) \varsigma_{3/2}(z=1) = 2.61238 V n_Q(T_E)$$

The temperature T_E can be derived as

$$k_B T_E = \frac{2\pi\hbar^2}{M} \left(\frac{N/V}{2.61238}\right)^{2/3}$$

Below T_E,

$$N_0(T) = N - N_e(T, z = 1) > 0$$

We define the molar mass weight as

$$M_A = mN_A$$

and the molar volume as

$$V_M = \frac{V}{N} N_A$$

Then the Einstein temperature is rewritten as

$$k_B T_E = \frac{2\pi\hbar^2}{M_A / N_A} \left(\frac{N_A / V_M}{2.61238}\right)^{2/3}$$

((**Note**))

$$\rho = \frac{M_A}{V_M} = \frac{M}{V} = \frac{M}{N}\frac{N}{V} = mn$$

Since $m = \dfrac{M_A}{N_A}$

$$n = \frac{\rho}{m} = \frac{M_A}{V_M}\frac{N_A}{M_A} = \frac{N_A}{V_M}$$

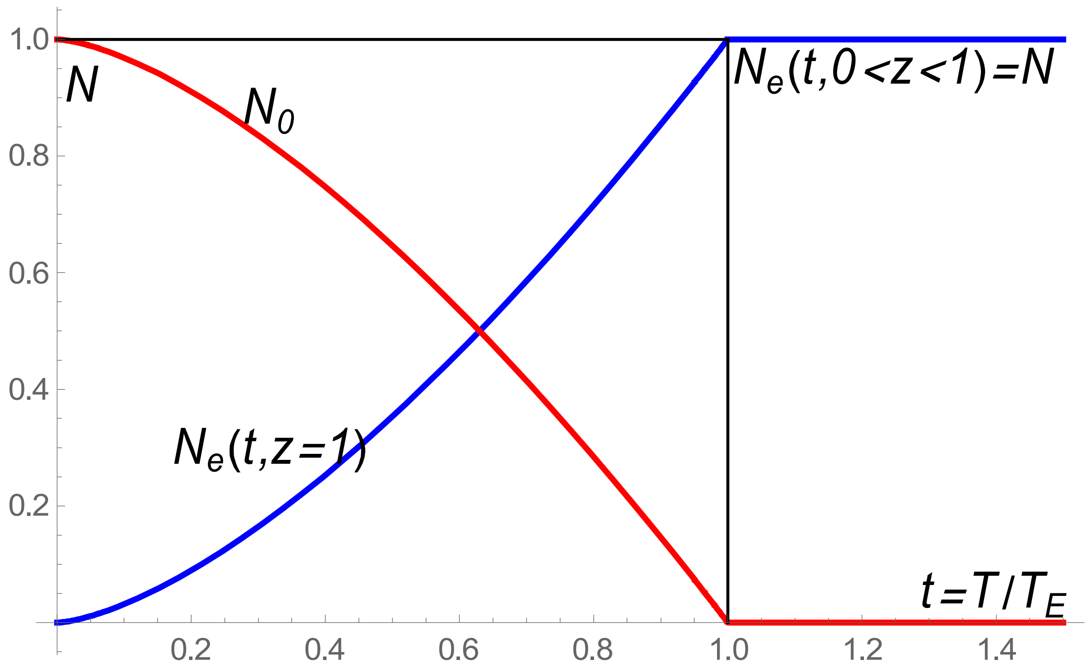

Fig. Temperature dependence of the thermally excited Bose particle density (blue solid line), $N_e(t, z=1)$ for t<1. The remaining density (N_0) occupies the ground state (red solid line). For t>1, $N_e(t, 0<z<1)=N$.

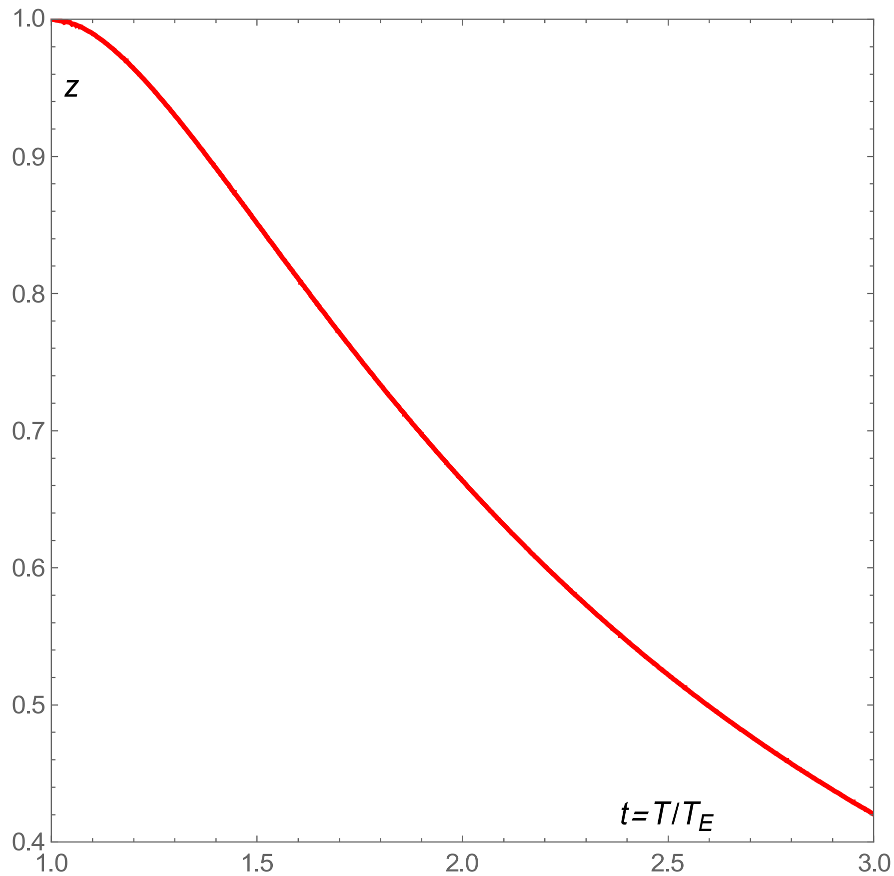

Fig. z vs the normalized temperature $t = T / T_E$ ($t > 1$). $z = e^{\beta\mu}$ (We use the ContourPlot to get this plot). $N_e(t, z) = N$.

((**Example**))

(a) Liquid ^{4}He;

$V_M = 27.6$ cm^3/mol, $M_A = 4$ g/mol.

$T_E = 3.13672$ K.

Note that the density ρ is given by

$$\rho = \frac{M_A}{V_M} = \frac{4}{27.6} = 0.145 \text{ g/cm}^3.$$

(b) Alkali metal Rb atom (which shows the Bose-Einstein condensation at extremely low temperatures);

$$\rho = \frac{M_A}{V_M} = 1.532 \text{ g/cm}^3. \qquad M_A = 85.4678 \text{ g/mol}$$

$$V_M = \frac{M_A}{\rho} = 55.78838 \text{ cm}^3\text{/mol}$$

$T_E = 91.8$ mK.

(c) Na atom

$$\rho = \frac{M_A}{V_M} = 0.968 \text{ g/cm}^3. \qquad M_A = 22.98977 \text{ g/mol}$$

$$V_M = \frac{M_A}{\rho} = 23.74976 \text{ cm}^3\text{/mol}$$

$T_E = 603.258$ mK.

((**Mathematica**))

```
Clear["Global`*"];

rule1 = {NA → 6.02214179 × 10^23, R → 8.314472, kB → 1.3806504 × 10^-23,
   h → 6.62606896 × 10^-34, ħ → 1.05457162853 × 10^-34, cm → 10^-2,
   g → 10^-3, VM → 27.6 cm^3, MA → 4 g};

TE = (2 π ħ^2)/(kB MA / NA) ((NA / VM)/2.61238)^(2/3) //. rule1

3.13672
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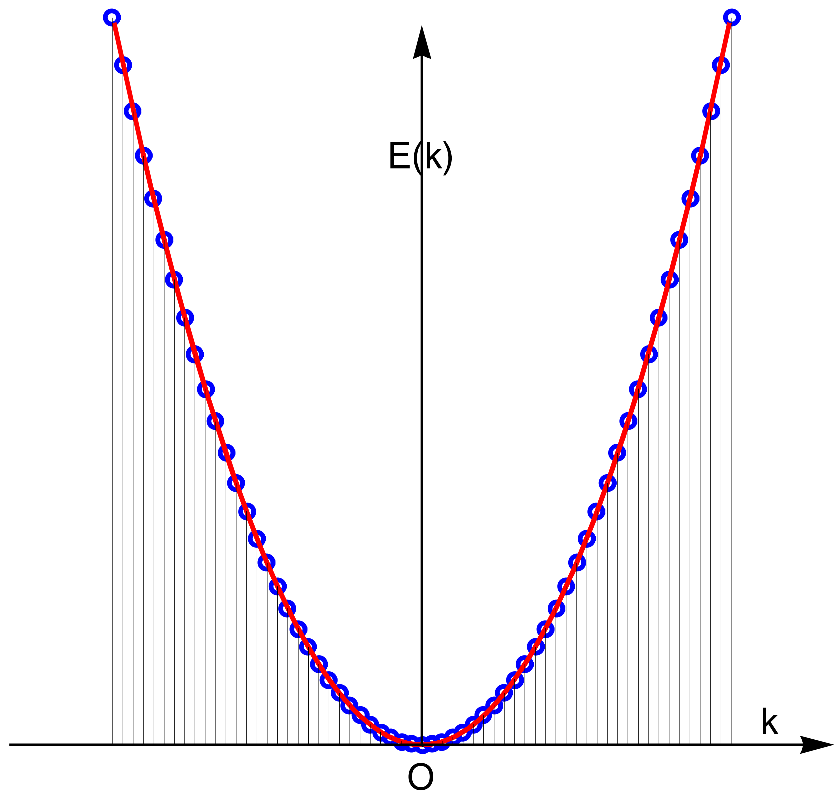
4. Physical meaning

In the limited space of the system, the energy of boson (as a single-particle) is quantized. At high temperature, each boson has an energy as a single-particle state. At $T = 0$ K, the boson is in the ground state ($\varepsilon = 0$, in Fig.). Suppose that N bosons are in the ground state of the single particle. This situation is very different from fermions. One fermion is at the ground state. Other fermions cannot stay in the ground state, because of the Pauli-exclusion principle. The second fermion will stay at the first excited state.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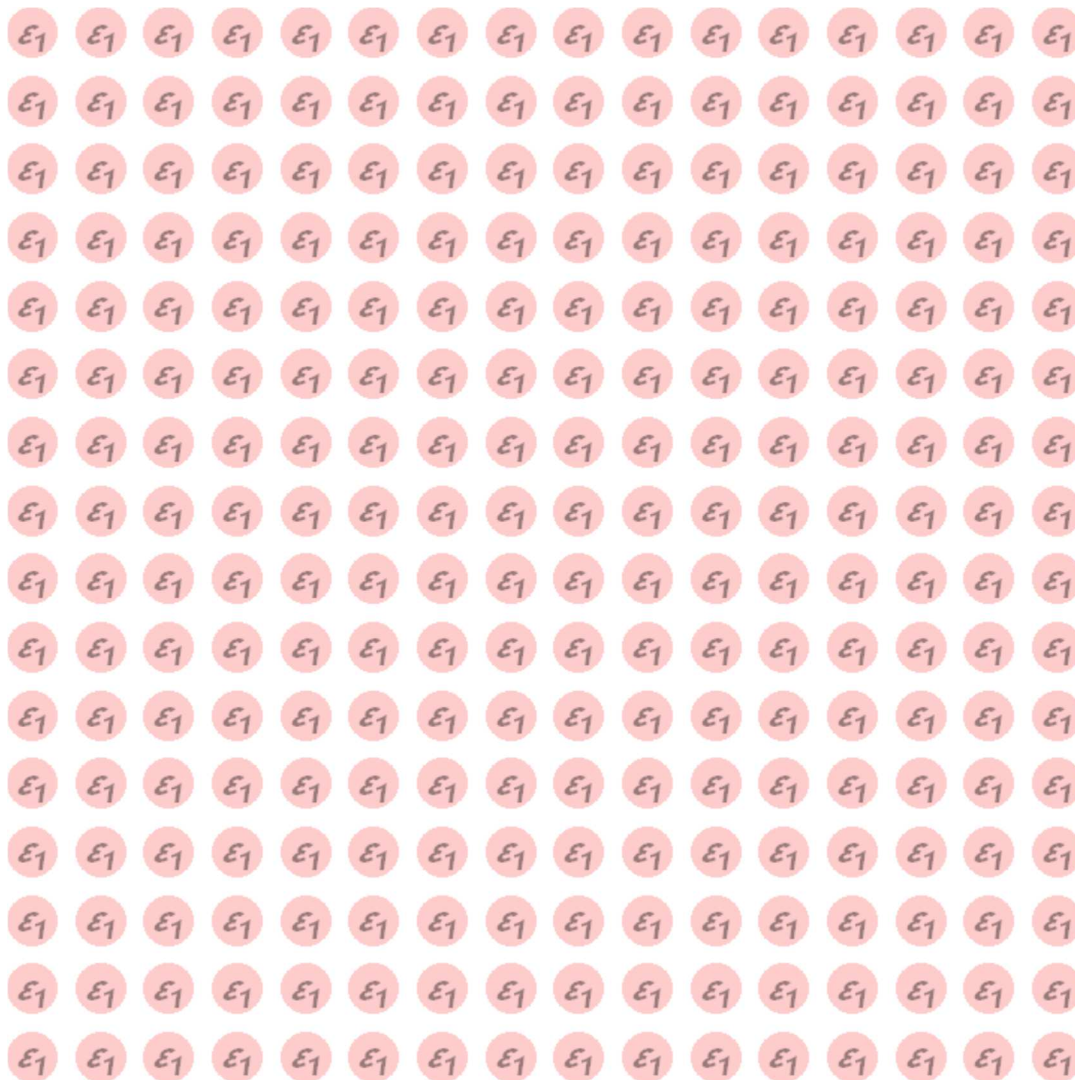

Fig. Bose-Einstein condensation. Each boson has the lowest energy of the single particle state. The de Broglie wave length beco0mes very large, forming a coherent state.

5. Order parameter $N_0(T)$

We consider the temperature dependence of the occupancy number $N_0(T)$ of the ground state below T_E.

$$N = N_0(T) + N_e(T, z = 1) = N_0(T) + Vn_Q(T)\varsigma_{3/2}(z = 1)$$

The Einstein temperature T_E is defined as

$$N = Vn_Q(T_E)\varsigma_{3/2}(z = 1) = 2.61238Vn_Q(T_E)$$

Then we get

$$N = N_0(T) + N\left(\frac{T}{T_E}\right)^{3/2}.$$

From this Eq., we have

$$\frac{N_0(T)}{N} = 1 - \left(\frac{T}{T_E}\right)^{3/2}$$

We make a plot of $\frac{N_0(T)}{N}$ as a function ot $t = T/T_E$. $\frac{N_0(T)}{N}$ becomes zero above T_E.

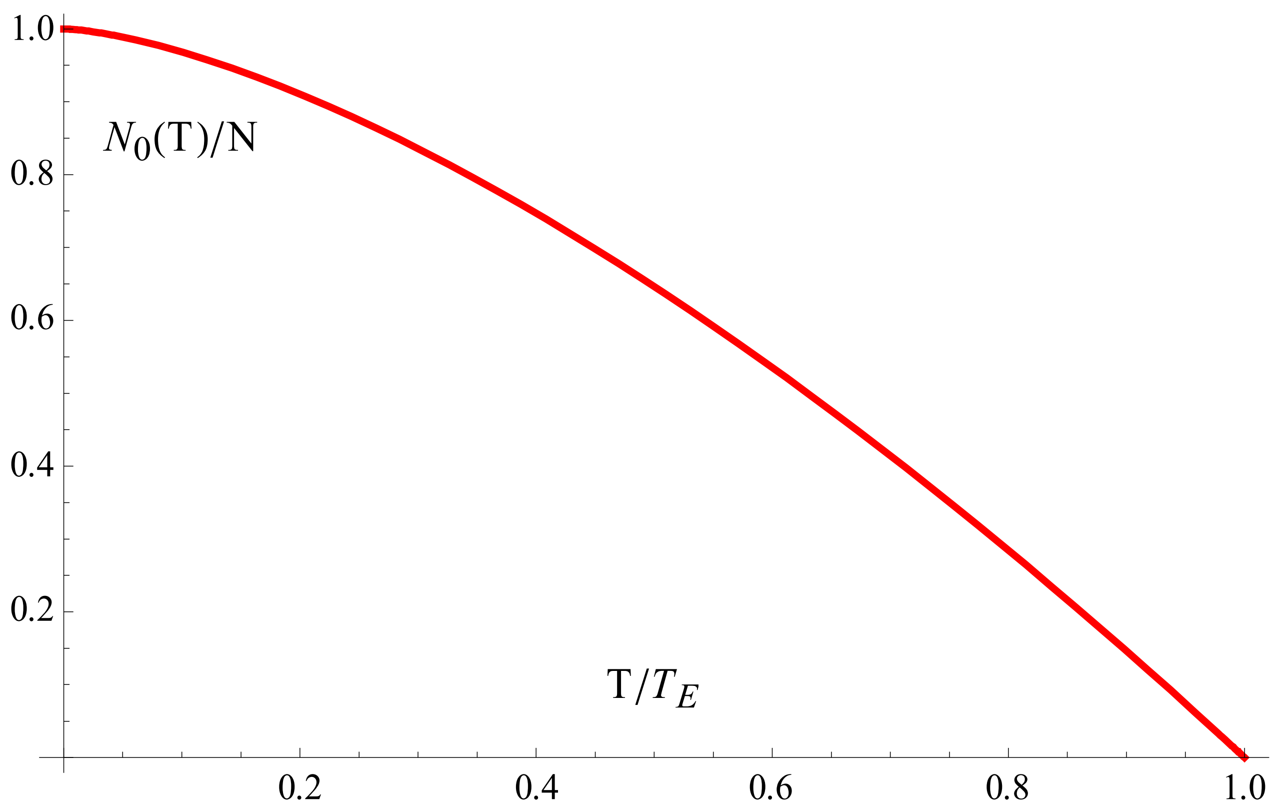

Fig. Plot of $N_0(T)/N$ as a function of reduced temperature $t = T/T_E$, showing the critical behavior in the vicinity of T_E.

6. The temperature dependence of z above T_E

$$N = N_e(T, z) = V n_Q(T) \varsigma_{3/2}(z)$$

At $T = T_{\mathrm{E}}$,

$$N = N_e(T_E, z = 1) = Vn_Q(T_E)\varsigma_{3/2}(z = 1) = Vn_Q(T_E)2.61238\ ,$$

Then we have

$$N = N_e(T, z) = Vn_Q(T)\varsigma_{3/2}(z)$$

and

$$N = Vn_Q(T_E)\varsigma_{3/2}(z = 1) = Vn_Q(T_E)2.61238$$

Thus we get

$$Vn_Q(T)\varsigma_{3/2}(z) = Vn_Q(T_E)2.61238$$

or

$$\varsigma_{3/2}(z) = (\frac{T_E}{T})^{3/2}2.61238 = 2.61238t^{-3/2}$$

since

$$n_Q(T) = \left(\frac{2\pi mk_BT}{h^2}\right)^{3/2}, \qquad t = \frac{T}{T_E}$$

From the numerical calculation (ContourPlot), the parameter z can be evaluated as a function of t

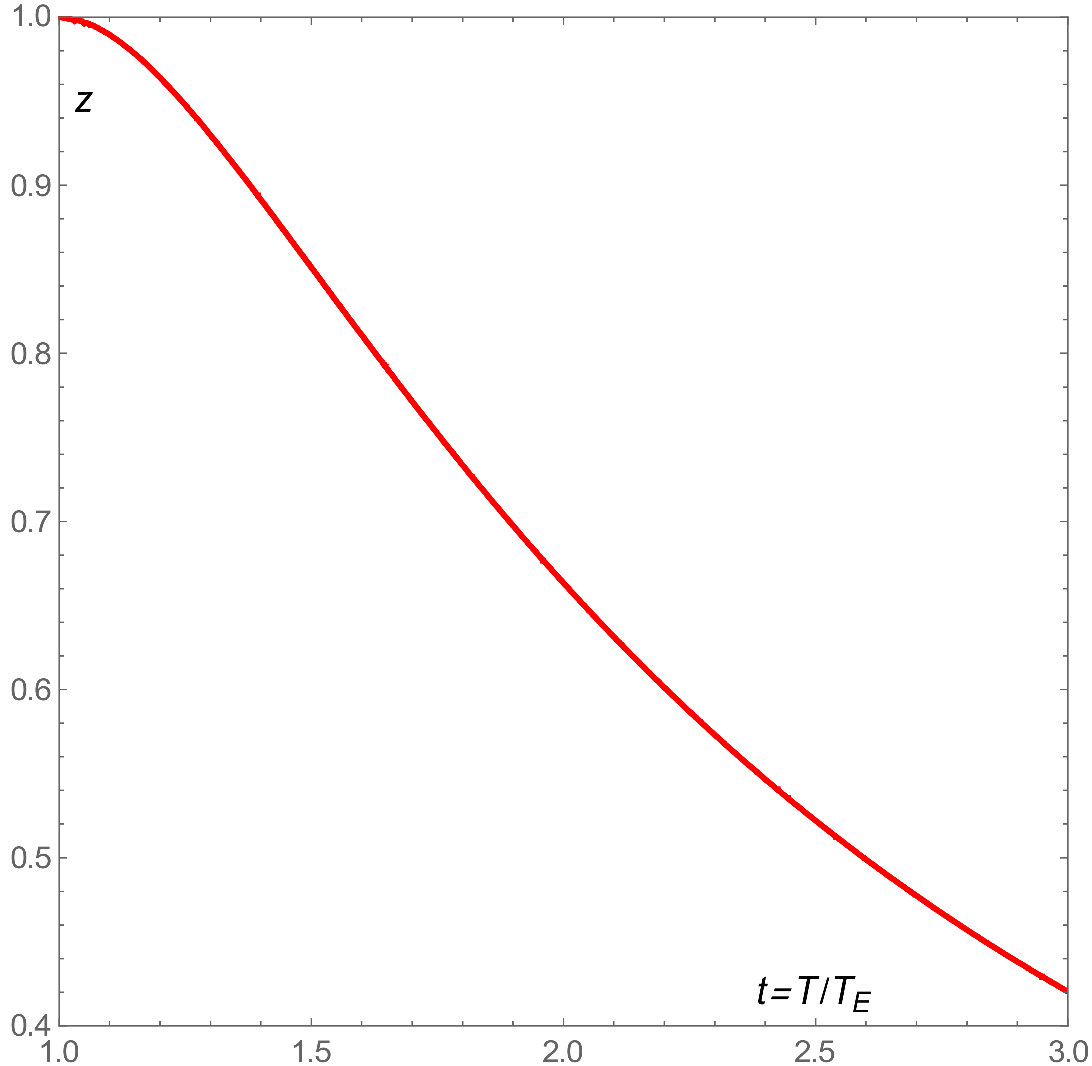

Fig. Plot of z vs a reduced temperature t above T_E. $z = e^{\beta\mu}$. The value z tends to $z = 1$ at $t = 1$.

Mathematica (ContourPlot): $\varsigma_{3/2}(z) = (\frac{T_E}{T})^{3/2} 2.61238 = 2.61238 t^{-3/2}$

7. Possibility of Bose-Einstein condensation in two dimensions

The density of states for the 2D system is given by

$$D_2(\varepsilon)d\varepsilon = \frac{L^2}{(2\pi)^2} 2\pi k dk \, .$$

Using the dispersion relation $\qquad \varepsilon = \frac{\hbar^2}{2m}k^2 \qquad$ or $\qquad k = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$

$$D_2(\varepsilon)d\varepsilon = \frac{L^2}{(2\pi)^2}2\pi\sqrt{\frac{2m\varepsilon}{\hbar^2}}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{\varepsilon}}d\varepsilon$$
$$= \frac{L^2}{4\pi}\frac{2m}{\hbar^2}d\varepsilon = \frac{mL^2}{2\pi\hbar^2}d\varepsilon$$

Suppose that all bosons are in the excited states,

$$N = N_e(T,z)$$

where

$$N_e(T,z) = \int_0^\infty D_2(\varepsilon)f(\varepsilon)d\varepsilon$$
$$= \frac{mL^2}{2\pi\hbar^2}\int_0^\infty f(\varepsilon)d\varepsilon$$
$$= \frac{mL^2}{2\pi\hbar^2}\int_0^\infty \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}$$
$$= \frac{mk_BTL^2}{2\pi\hbar^2}\int_0^\infty \frac{dx}{\frac{1}{z}e^x - 1}$$
$$= \frac{mk_BTL^2}{2\pi\hbar^2}\int_0^\infty \frac{ze^{-x}dx}{1-ze^{-x}}$$

with

$$z = e^{\beta\mu}, \qquad x = \beta\varepsilon .$$

Noting that

$$\int_0^\infty \frac{ze^{-x}dx}{1-ze^{-x}} = -\ln(1-z) = \ln(\frac{1}{1-z})$$

we get the number density as

$$n_e(T,z) = \frac{N_e(T,z)}{L^2} = \frac{mk_BT}{2\pi\hbar^2}\ln(\frac{1}{1-z}) = n_{2D}(T)\ln(\frac{1}{1-z})$$

where

$$n_{2D}(T) = \frac{mk_B T}{2\pi\hbar^2}.$$

Since $n_e(T, z) = n$ =constant, we have

$$n = n_{2D}(T)\ln(\frac{1}{1-z})$$

or

$$\frac{n}{\ln(\frac{1}{1-z})}|_{z\to 1} = \frac{mk_B T_E}{2\pi\hbar^2}$$

When $z \to 1$, we have $T_E \to 0$. So we do not have any finite critical temperature. In other word, the Bose-Einstein does not occur in the 2D system.

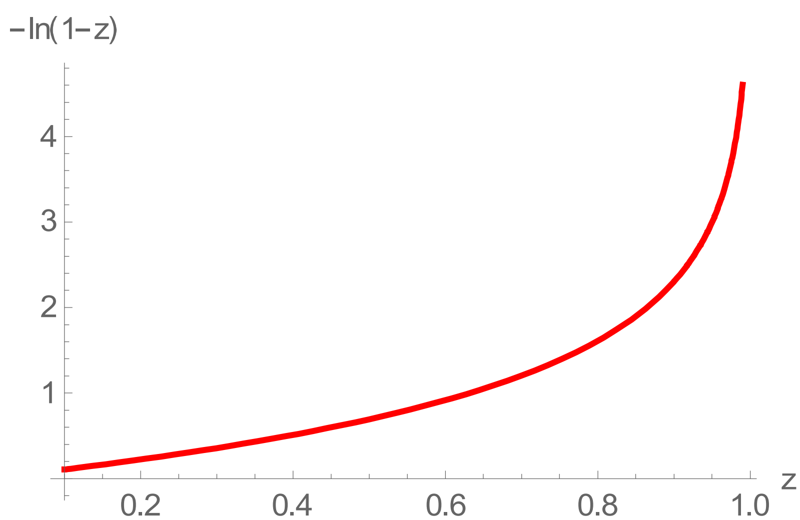

Fig. Plot of $-\ln(1-z)$ as a function of z. It diverges at $z = 1$.

In other words, there is no finite critical temperature for the Bose-Einstein condensation in 2D systems.

In conclusion

3D system: Bose-Einstein condensation

2D system: No condensation occurs.

The phenomena of the superconductivity and superfluidity are observed only for the 3D system.