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 $\beta = \dfrac{1}{k_B T}$ 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.

((**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

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

The number *N* (fixed) is expressed by

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

where $N_e(T)$ 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

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

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

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

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

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

Here we have

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

and

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

where

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

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

$$N_e(T) = \frac{V}{4\pi^2} (\frac{2M}{\hbar^2})^{3/2} \int_0^\infty k_B T dx \frac{(k_B T)^{1/2} \sqrt{x}}{\frac{1}{\lambda} e^x - 1} = \frac{V}{4\pi^2} (4\pi)^{3/2} (\frac{M k_B T}{2\pi\hbar^2})^{3/2} \int_0^\infty dx \frac{\sqrt{x}}{\frac{1}{\lambda} e^x - 1}$$

Since the integral (for λ<1) is obtained as

$$I = \int_0^\infty dx \frac{\sqrt{x}}{\frac{1}{\lambda}e^x - 1} = \int_0^\infty dx \frac{\lambda e^{-x}\sqrt{x}}{1-\lambda e^{-x}} = \frac{\sqrt{\pi}}{2}\varsigma(\frac{3}{2},\lambda),$$

Then we get

$$N_e(T) = \frac{V}{4\pi^2}(4\pi)^{3/2}(\frac{Mk_BT}{2\pi\hbar^2})^{3/2}\frac{\sqrt{\pi}}{2}\varsigma_{3/2}(\lambda) = Vn_Q(T)\varsigma_{3/2}(\lambda)$$

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

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

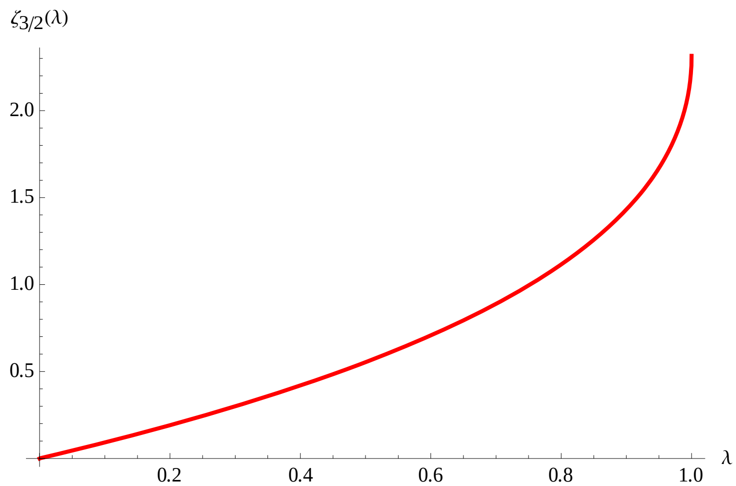

Fig. Plot of $\varsigma_{3/2}(\lambda)$ as a function of λ. $\varsigma_{3/2}(\lambda = 1)$ = 2.61238

3. Einstein-Condensation temperature T_E

The temperature T_E at which λ = 1 is called the critical temperature for Bose condensation

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

or

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

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

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

((Example))
For 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

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

For Rb atom;

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

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

$T_E = 91.8$ mK.

For 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. Order parameter $N_0(T)$

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

$$N = N_0(T) + N_e(T) = \frac{1}{\frac{1}{\lambda} - 1} + V n_Q(T) \varsigma_{3/2}(\lambda)$$

with $\lambda = e^{\beta\mu} < 1$ (μ should be negative). Since N is fixed, the temperature dependence of λ can be derived from the above equation.

For $\lambda = 1$, $N_0(T) \to N$. The Einstein temperature T_E is defined as

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

Then we get

$$N = \frac{\lambda}{1-\lambda} + N\left(\frac{T}{T_E}\right)^{3/2} \frac{\varsigma_{3/2}(\lambda)}{\varsigma_{3/2}(\lambda=1)}.$$

From this Eq., we have

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

Here we define

$$f_N(\lambda) = \frac{1}{N}\frac{\lambda}{1-\lambda}$$

and

$$g_N(\lambda) = \left(\frac{T}{T_E}\right)^{3/2} \frac{\varsigma_{3/2}(\lambda)}{\varsigma_{3/2}(\lambda=1)},$$

which is independent of *N*. The above equation reduces to

$$1 = f_N(\lambda) + g_N(\lambda)$$

(i) $T<T_E$.

Near $\lambda = 1$, there is an intersection of $g_N(\lambda)$ and $f_N(\lambda)$.

At $\lambda = 1$,

$$g_N(\lambda=1) = \left(\frac{T}{T_E}\right)^{3/2}.$$

Then

$$\begin{aligned} N &= N_0(T) + N_e(T) \\ &= N_0(T) + N g_N(\lambda=1) \end{aligned}$$

or

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

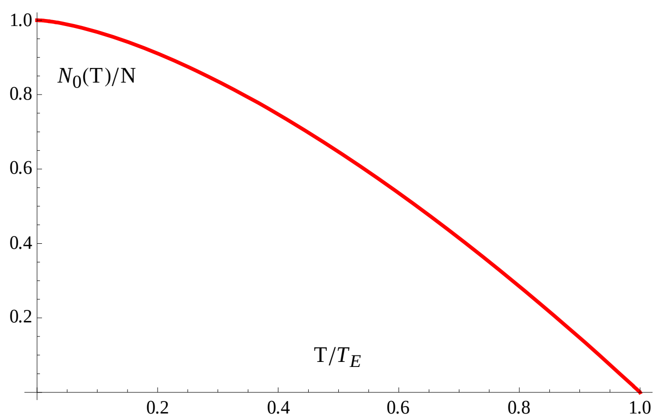


Fig. Plot of $N_0(T)/N$ as a function of reduced temperature T/T_E.

(ii) $T>T_E$.

$$f_N(\lambda) = 0\,, \qquad g_N(\lambda) = 1$$

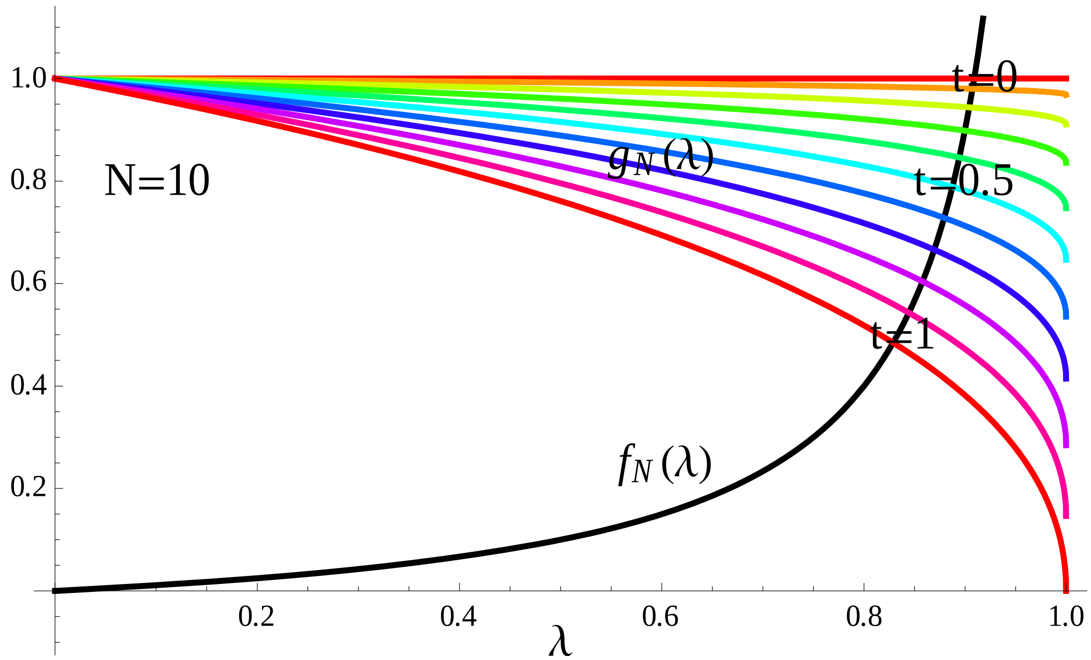
or

$$N_e(T) = Ng_N(\lambda = 1) = N\,, \qquad N_O(T) = 0$$

5. Numerical results (I)

We calculate $f_N(\lambda)$ and $g_N(\lambda)$ as a function of λ to determine the value of λ where two curves intersect.

(a) $N = 10$



Fig, Plot of $f_N(\lambda)$ and $g_N(\lambda)$ as a function of λ. $N = 10$. The parameter t (= T/T_E)

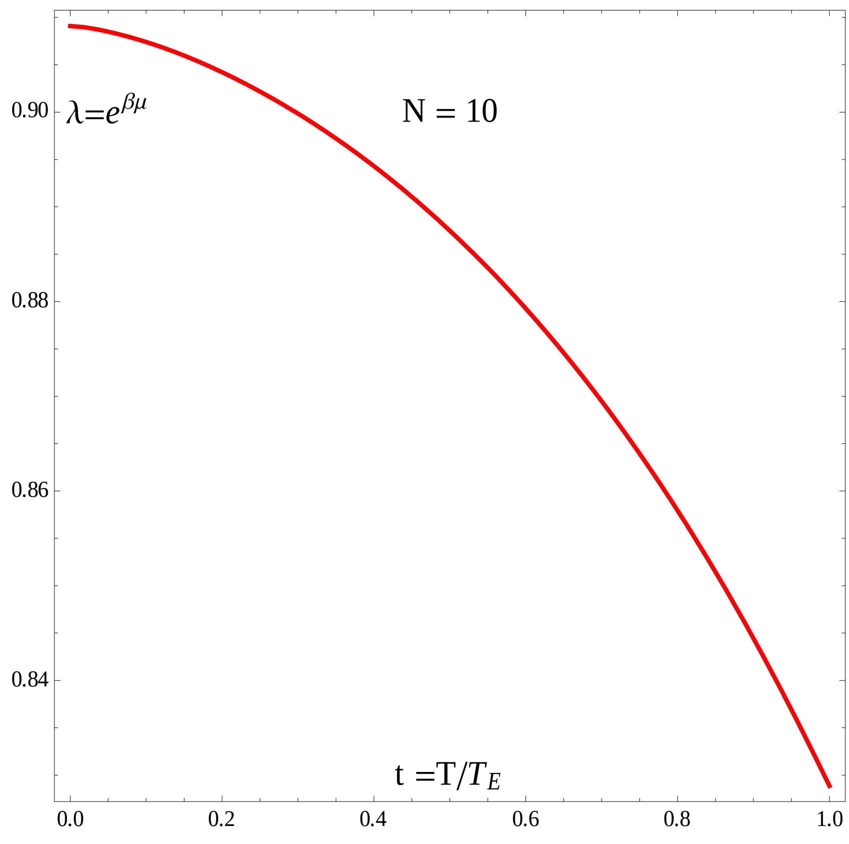
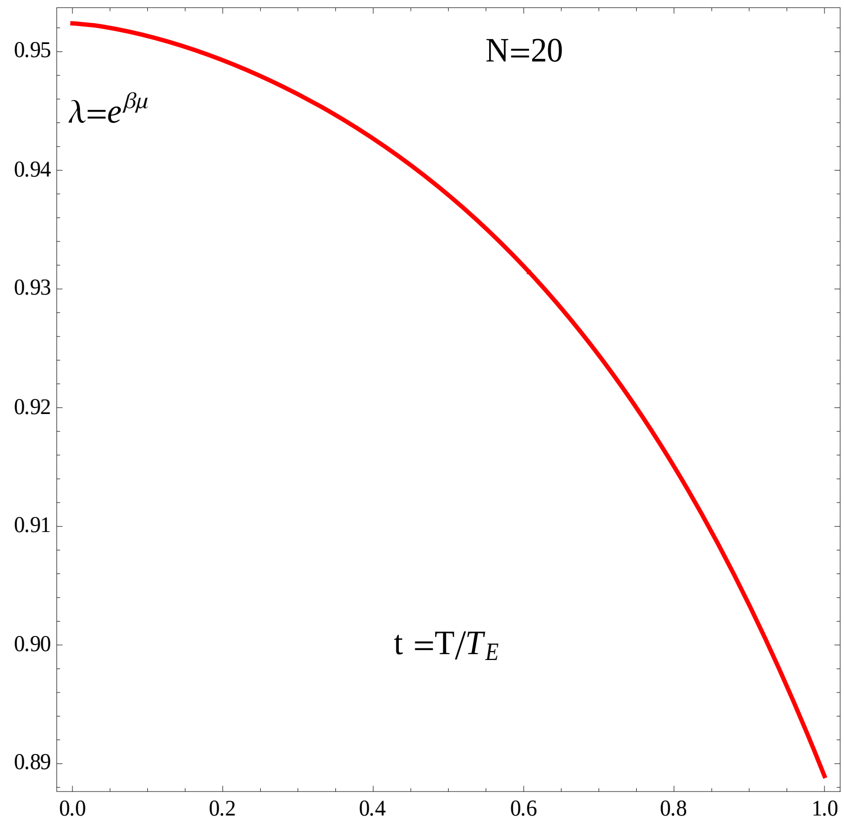
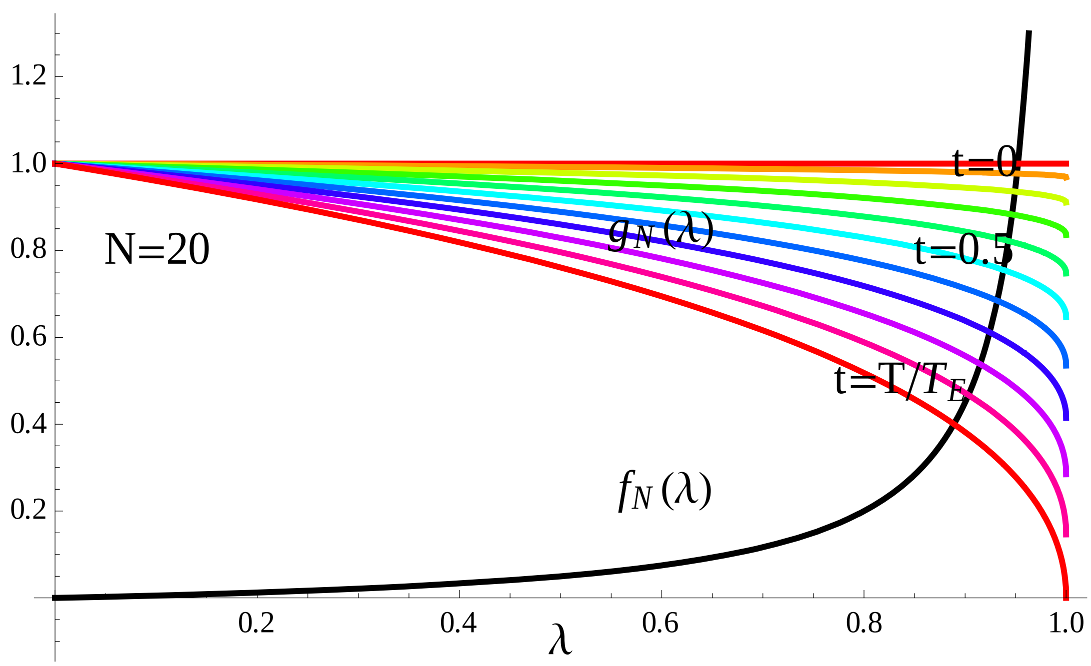


Fig. Plot of $\lambda = e^{\beta\mu}$ vs t (= T/T_E). $N = 10$

(b) $N = 20.$

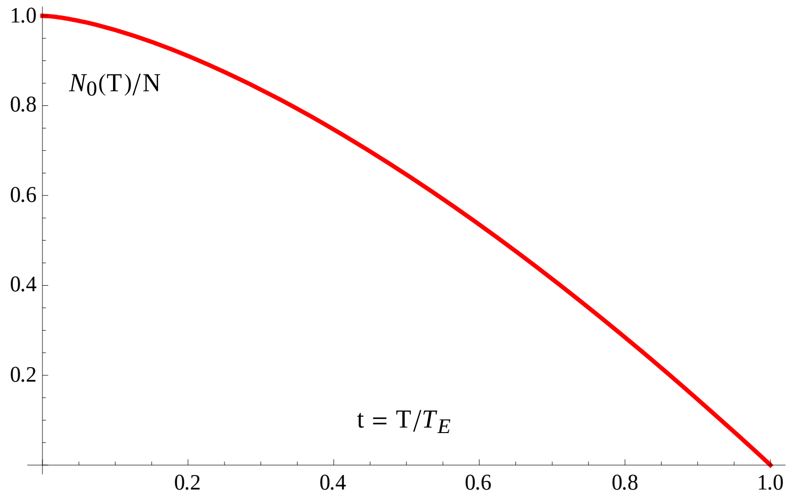


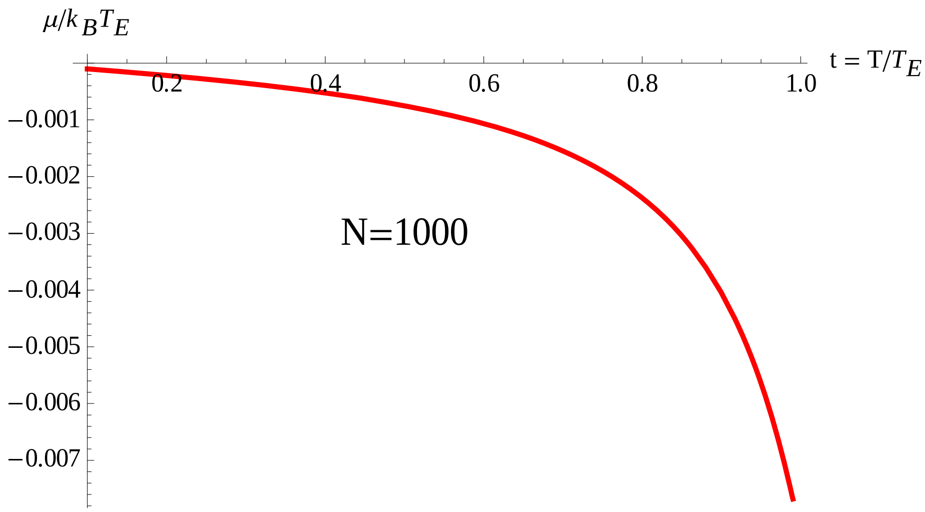
0.95
0.94
0.93
0.92
0.91
0.90
0.89
N=20
λ=e^βμ
t =T/T_E
0.0
0.2
0.4
0.6
0.8
1.0

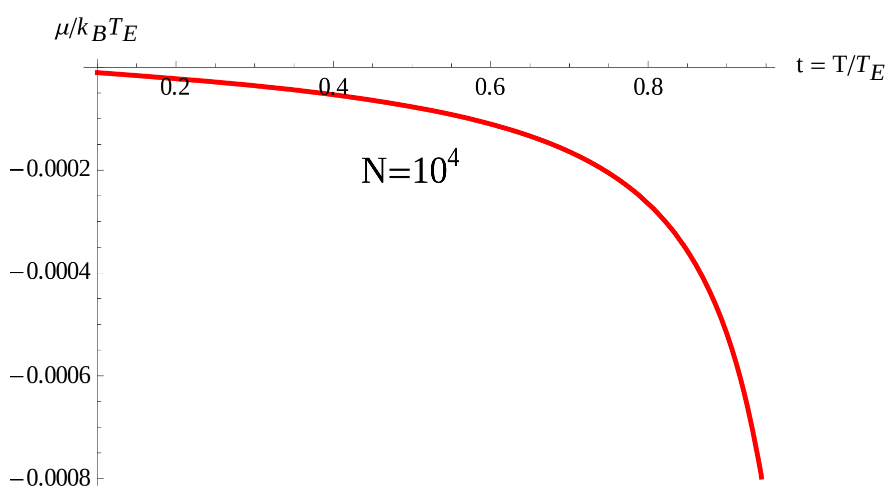


1.2
1.0
0.8
0.6
0.4
0.2
N=20
g_N(λ)
f_N(λ)
t=0
t=0.5
t=T/T_E
0.2
0.4
0.6
0.8
1.0
λ

6. Numerical results (II)







7. Possibility of Bose-Einstein condensation in two dimensions

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

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

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

$$= \frac{L^2}{4\pi} \frac{2m}{\hbar^2} d\varepsilon = \frac{mL^2}{2\pi\hbar^2} d\varepsilon$$

$$N = N_0 + N_e$$

$$N_e = \int_0^\infty D_2(\varepsilon) f(\varepsilon) d\varepsilon = \frac{mL^2}{2\pi\hbar^2} \int_0^\infty f(\varepsilon) d\varepsilon$$

$$= \frac{mL^2}{2\pi\hbar^2} \int_0^\infty \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} - 1} = \frac{mL^2}{2\pi\hbar^2} k_B T \int_0^\infty \frac{dx}{\frac{1}{\lambda}e^x - 1} = \frac{mL^2}{2\pi\hbar^2} k_B T \int_0^\infty \frac{\lambda e^{-x} dx}{1 - \lambda e^{-x}}$$

and

$$N_0 = \frac{1}{\frac{1}{\lambda} - 1} = \frac{\lambda}{1 - \lambda}$$

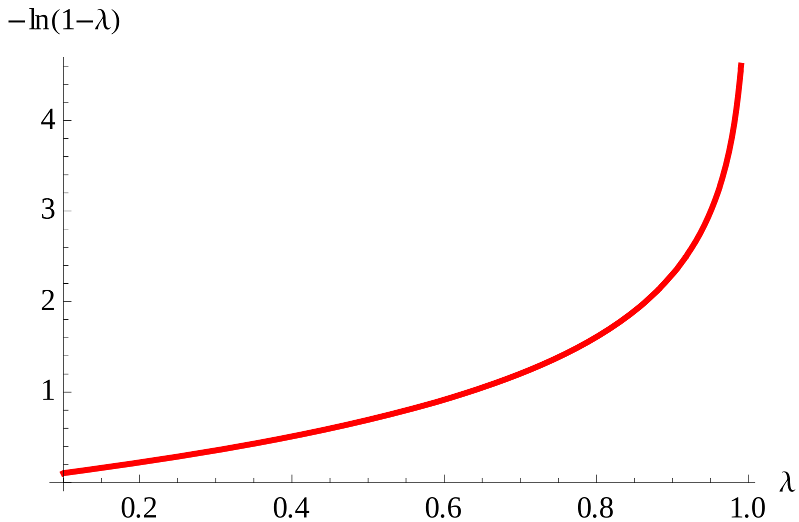
where

$$\lambda = e^{\beta\mu},$$

with $x = \beta\varepsilon$,

We note that

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



Then we have

$$1 = \frac{1}{N}\frac{\lambda}{1-\lambda} + \frac{mL^2}{2\pi\hbar^2 N} k_B T \ln(\frac{1}{1-\lambda})$$

or

$$1 - \frac{1}{N}\frac{\lambda}{1-\lambda} = \frac{mL^2}{2\pi\hbar^2 N} k_B T \ln(\frac{1}{1-\lambda}),$$

or

$$g = (1 - \frac{1}{N}\frac{\lambda}{1-\lambda})\frac{1}{\ln(\frac{1}{1-\lambda})} = \frac{mL^2}{2\pi\hbar^2 N} k_B T$$

We make a plot of g vs λ in the very vicinity of $\lambda = 1$ for $\lambda<1$, where $N = 10^6$. The value of g decreases as approaches $\lambda = 1$ from the lower side of λ, but does not reduces to zero. The right-hand side should be equal to zero when the critical temperature is finite and N becomes extremely large. In fact, the curve (g vs λ) does not intersect with the $g = 0$ line, which means that the Bose-Einstein condensation does not occur in the 2D system.

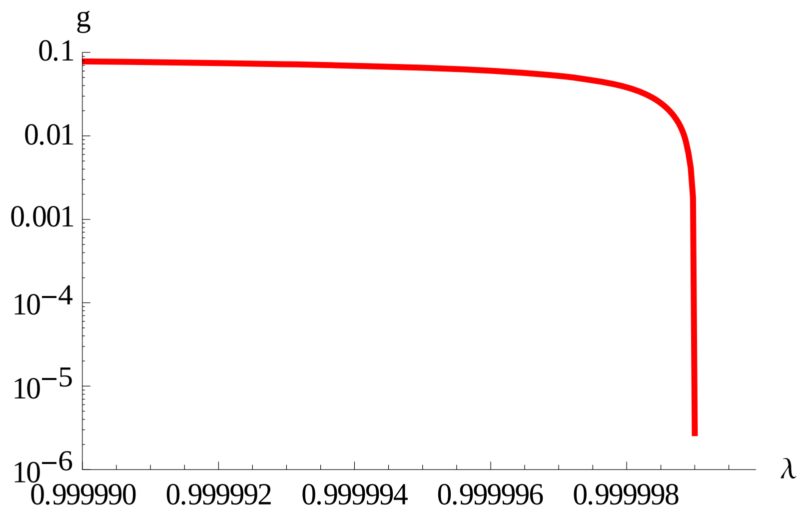


Fig. Plot of g vs λ, where $N = 10^6$.

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.

8. Heat capacity

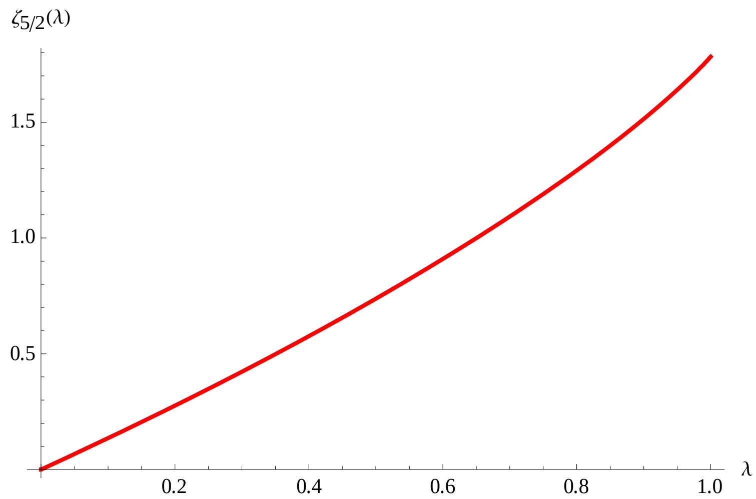
The total energy is given by

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

$$= \frac{V}{4\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\frac{1}{\lambda}e^{\beta\varepsilon} - 1} = \frac{V}{4\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} \int_0^\infty d\varepsilon \frac{\varepsilon^{3/2}}{\frac{1}{\lambda}e^{\beta\varepsilon} - 1}$$

$$= \frac{V}{4\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} (k_B T)^{5/2} \int_0^\infty dx \frac{x^{3/2}}{\frac{1}{\lambda}e^{x} - 1} = \frac{V}{4\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} (k_B T)^{5/2} \frac{3\sqrt{\pi}}{4} \varsigma_{5/2}(\lambda)$$

Note that there is no contribution from $\varepsilon = 0$ state.



Plot of $\varsigma_{5/2}(\lambda)$ as a function of λ. $\varsigma_{5/2}(\lambda = 1) = 1.34149$.

Then the ratio is given by

$$\frac{E}{N_e(T)} = \frac{\frac{V}{4\pi^2}(\frac{2M}{\hbar^2})^{3/2}(k_B T)^{5/2}\frac{3\sqrt{\pi}}{4}\varsigma_{5/2}(\lambda)}{\frac{V}{4\pi^2}(4\pi)^{3/2}(\frac{Mk_B T}{2\pi\hbar^2})^{3/2}\frac{\sqrt{\pi}}{2}\varsigma_{3/2}(\lambda)} = \frac{3}{2}k_B T\frac{\varsigma_{5/2}(\lambda)}{\varsigma_{3/2}(\lambda)}$$

Here we note that

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

where

$$N_e(T) = N \qquad \text{for } T>T_E,$$

$$N_e(T) = N\left(\frac{T}{T_E}\right)^{3/2} \qquad \text{for } T<T_E.$$

(i) $T<T_E$,
E is given by

$$E = \frac{3}{2} k_B T N_e(T) \frac{\varsigma_{5/2}(\lambda)}{\varsigma_{3/2}(\lambda)} |_{\lambda=1} = \frac{3}{2} k_B T \left(\frac{1.34149}{2.61238} \right) N_e(T)$$

$$= \frac{3}{2} k_B T (0.513513) N_e(T)$$

Using the expression of $N_e(T)$, we get

$$E = \frac{3}{2} k_B T (0.513513) N \left(\frac{T}{T_E} \right)^{3/2},$$

The heat capacity C_V is obtained as

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V = \frac{3}{2} N k_B (0.513513) \frac{5}{2} \left(\frac{T}{T_E} \right)^{3/2} = \frac{3}{2} N k_B (1.2837825) t^{3/2}$$

for $T<T_E$, where t is the reduced temperature,

$$t = \frac{T}{T_E}.$$

(ii) $T>T_E$,
$N_e(T)$ is given by

$$N = N_e(T) = V (\frac{M k_B T}{2\pi\hbar^2})^{3/2} \varsigma_{3/2}(\lambda)$$

At $T = T_E$,

$$N = N_e(T_E) = V (\frac{M k_B T_E}{2\pi\hbar^2})^{3/2} \varsigma_{3/2}(\lambda = 1) = V (\frac{M k_B T_E}{2\pi\hbar^2})^{3/2} 2.61238,$$

Then we have

$$N = N_e(T) = V (\frac{M k_B T}{2\pi\hbar^2})^{3/2} \varsigma_{3/2}(\lambda) = V (\frac{M k_B T_E}{2\pi\hbar^2})^{3/2} 2.61238$$

or

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

From the numerical calculation, the parameter λ can be evaluated as a function of t

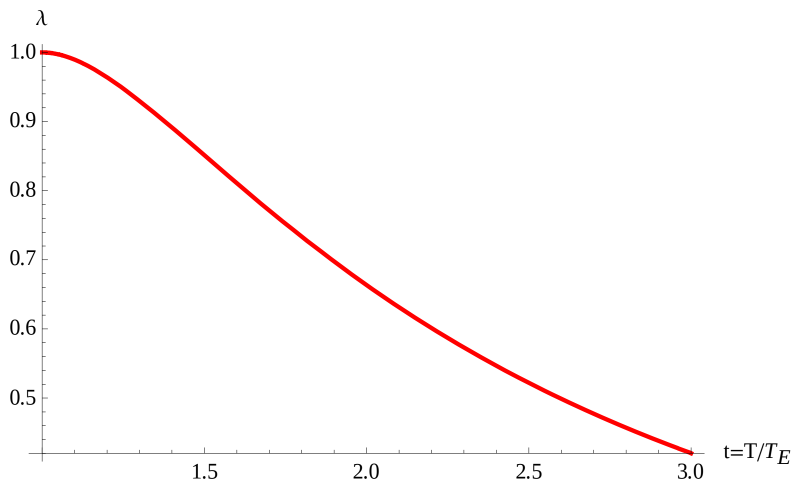


Fig. Plot of λ vs a reduced temperature t above T_E.

Then the total energy is given by

$$E = \frac{3}{2} N k_B T \frac{\varsigma_{5/2}(\lambda)}{\varsigma_{3/2}(\lambda)} = \frac{3}{2} N k_B T_E t \frac{\varsigma_{5/2}(\lambda(t))}{\varsigma_{3/2}(\lambda(t))}$$

The heat capacity C_V is evaluates as

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{3}{2} N k_B \frac{\partial}{\partial t}[t \frac{\varsigma_{5/2}(\lambda(t))}{\varsigma_{3/2}(\lambda(t))}]$$

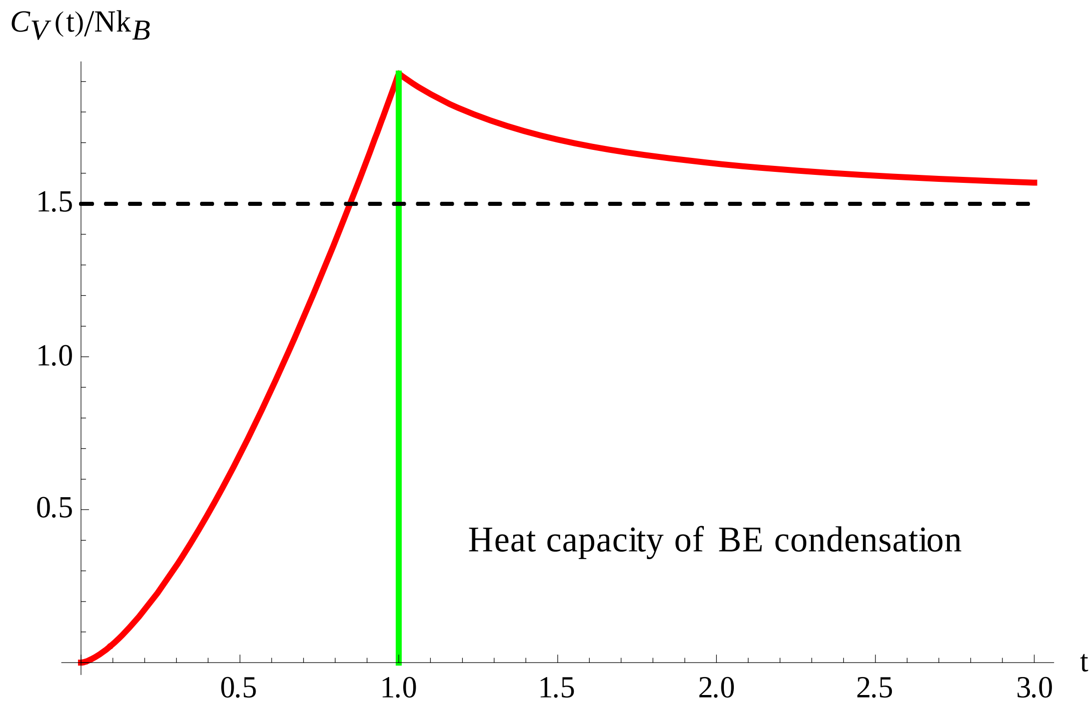


Fig. Normalized heat capacity vs a reduced temperature t (= T/T_E).

((Mathematica))

Heat capacity of the Bose-Einstein condensation

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

k1[t_] := PolyLog[3/2, λ] - PolyLog[3/2, 1]/t^(3/2);

Lamda[t_] := Module[{eq1, eq2, λ1},
   eq1 = FindRoot[k1[t] == 0, {λ, 0.1, 1}]; λ1 = λ /. eq1[[1]]];
```

Interpolation and its derivative

```
E1[t_] := t PolyLog[5/2, Lamda[t]]/PolyLog[3/2, Lamda[t]];

g1 = Table[{t, E1[t]}, {t, 1, 10, 0.01}]; g11 = Interpolation[g1];
CU = g11';
```

CU :heat capacity normalized by $\frac{3}{2}$ Nk_B for T>TE

CD: heat capacity normalized by $\frac{3}{2}$ Nk_B for T<TE

```
CD[t_] := 1.2837825 t^(3/2);
```

```
CDU = Which[0 < t < 1, CD[t], t > 1, CU[t]];
p1 = Plot[CDU, {t, 0, 3}, PlotStyle → {Red, Thick},
   AxesLabel → {"t", "C_V (t) / (3/2 Nk_B) "}];
p2 =
 Graphics[
  {Text[Style["Heat capacity of BE condensation", Black, 12],
    {2.5, 0.4}], Green, Thick, Line[{{1, 0}, {1, CD[1]}}],
   Dashed, Thin, Black, Line[{{0, 1}, {3, 1}}] }];
Show[p1, p2]
```