Consider an ideal Bose gas of free, non-relativistic particles in a box in 3 dimensions. The particles have an internal degree of freedom that can take only one of two energy values, the ground state with $\varepsilon_0 = 0$, and an excited state with $\varepsilon_1 > 0$. Determine the Bose-Einstein condensation temperature T_c of the gas as a function of ε_1. You only need to write the equation by which one could in principle solve for T_c.

Then, for the particular case that $\varepsilon_1/k_B T \gg 1$, show that,

$$\frac{T_c}{T_{c0}} = 1 - \frac{2e^{-\varepsilon_1/k_B T_{c0}}}{3\zeta(\frac{3}{2})}$$

where T_{c0} is the transition temperature when ε_1 is infinite, and ζ is the Riemann zeta function.

Hint: Recall that the standard functions for bosons are

$$g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty dy \frac{y^{n-1}}{z^{-1}e^y - 1} = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^n} \quad \text{and that} \quad \Gamma(n+1) = n\Gamma(n) \text{ and } \Gamma(1/2) = \sqrt{\pi}$$

4) $n = \frac{N}{V} = \frac{1}{V} \sum_{\vec{k}} \sum_{i=0,1} \frac{1}{z^{-1} e^{\beta(\varepsilon_k + \varepsilon_i)} - 1}$

wavevectors   internal degree of freedom

where $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ is the kinetic part of the energy

$\varepsilon_i = 0, \varepsilon_1$ is the energy of the internal degree of freedom

ground state is $\vec{k} = 0, i = 0$ with energy $\varepsilon_{min} = 0$

make the continuum approximation for the sum on $\vec{k}$, splitting off the ground state

$$n = n_0 + \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3k \sum_{i=0,1} \frac{1}{z^{-1} e^{\beta\left(\frac{\hbar^2 k^2}{2m} + \varepsilon_i\right)} - 1}$$

$$= n_0 + \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3k \frac{1}{z^{-1} e^{\frac{\beta\hbar^2 k^2}{2m}} - 1} \quad i=0 \text{ term}$$

$$+ \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3k \frac{1}{z^{-1} e^{\beta\varepsilon_1} e^{\frac{\beta\hbar^2 k^2}{2m}} - 1} \quad i=1 \text{ term}$$

convert to spherical coordinates $\int_{-\infty}^{\infty} d^3k \to 4\pi \int_0^{\infty} dk\, k^2$

$$n = n_0 + \frac{4\pi}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2}{z^{-1} e^{\frac{\beta\hbar^2 k^2}{2m}} - 1}$$

$$+ \frac{4\pi}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2}{z^{-1} e^{\beta\varepsilon_1} e^{\frac{\beta\hbar^2 k^2}{2m}} - 1}$$

let $y = \frac{\beta \hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2my}{\beta\hbar^2}}$

$$dy = \frac{2\beta\hbar^2 k\,dk}{2m}$$

so $$dk\,k^2 = \frac{2m}{2\beta\hbar^2}\sqrt{\frac{2m}{\beta\hbar^2}}\sqrt{y}\,dy$$

$$= \frac{1}{2}\left(\frac{2m}{\beta\hbar^2}\right)^{3/2}\sqrt{y}\,dy$$

$$n = n_0 + \frac{1}{2\pi^2}\frac{1}{2}\left(\frac{2m}{\beta\hbar^2}\right)^{3/2}\left[\int_0^\infty dy\,\frac{y^{1/2}}{z^{-1}e^{y}-1} + \int_0^\infty dy\,\frac{y^{1/2}}{z^{-1}e^{\beta\varepsilon_1}e^{y}-1}\right]$$

$$= n_0 + \frac{1}{\lambda^3}\frac{2}{\sqrt{\pi}}\int dy\,\frac{y^{1/2}}{z^{-1}e^{y}-1}$$

$$+ \frac{1}{\lambda^3}\frac{2}{\sqrt{\pi}}\int dy\,\frac{y^{1/2}}{z^{-1}e^{\beta\varepsilon_1}e^{y}-1}$$

where $\lambda^2 = \left(\frac{h^2}{2\pi m k_B T}\right)$ gives thermal wavelength

Standard function is

$$g_{3/2}(z) = \frac{2}{\sqrt{\pi}}\int_0^\infty dy\,\frac{y^{1/2}}{z^{-1}e^{y}-1}$$

So

$$\boxed{n = n_0 + \frac{g_{3/2}(z)}{\lambda^3} + \frac{g_{3/2}\left(ze^{-\beta\varepsilon_1}\right)}{\lambda^3}}$$

For fixed n, the goal is to solve the above for $n_0 = 0$ and $z < 1$ for normal state, $n_0 \geq 0$ and $z = 1$ BEC

At the Bose Einstein condensation temperature T_c we have $\mu = \varepsilon_{min} = 0$ so $z = 1$ and $n_0 = 0$

when $z = 1$, $z e^{-\beta \varepsilon_1} < 1$

at T_c exactly, $\beta_c = 1/k_B T_c$

(*) $$\boxed{n = \frac{g_{3/2}(1)}{\lambda_c^3} + \frac{g_{3/2}(e^{-\beta_c \varepsilon_1})}{\lambda_c^3}}$$

in principle, solve to determine λ_c and hence T_c

where $\lambda_c = \left(\frac{h^2}{2\pi m k_B T_c} \right)^{1/2}$ is thermal wavelength

$$g_{3/2}(1) = \zeta(3/2) \text{ Reimann zeta function}$$

Now when $\varepsilon_1 \to \infty$, $e^{-\beta_c \varepsilon} \to 0$, and $g_{3/2}(0) = 0$
so in this case T_{c0} determined by

(**) $$n = \frac{\zeta(3/2)}{\lambda_{c0}^3} \qquad \lambda_{c0} = \left(\frac{h^2}{2\pi m k_B T_{c0}} \right)^{1/2}$$

So when $\varepsilon_1/k_B T \gg 1$ then $e^{-\beta \varepsilon} \ll 1$

can approximate $g_{3/2}(z) \simeq z + \frac{z^2}{2^{3/2}} + \cdots$

we only need to keep the smallest term.

From (*) at $T = T_c$ for finite $\varepsilon_1 \gg k_B T_c$

$$n = \frac{\zeta(3/2)}{\lambda_{c0}^3}\left(\frac{T_c}{T_{c0}}\right)^{3/2} + \frac{e^{-\beta_c \varepsilon_1}}{\lambda_{c0}^3}\left(\frac{T_c}{T_{c0}}\right)^{3/2}$$

since $\lambda_c = \left(\dfrac{h^2}{2\pi m k_B T_c}\right)^{1/2} = \lambda_{c0}\left(\dfrac{T_{c0}}{T_c}\right)^{1/2}$

So

$$\frac{n\lambda_{c0}^3}{\zeta(3/2)} = \left[1 + \frac{e^{-\beta_c \varepsilon_1}}{\zeta(3/2)}\right]\left(\frac{T_c}{T_{c0}}\right)^{3/2}$$

From (**) we have $n\lambda_{c0}^3/\zeta(3/2) = 1$

So $$1 = \left[1 + \frac{e^{-\beta_c \varepsilon_1}}{\zeta(3/2)}\right]\left(\frac{T_c}{T_{c0}}\right)^{3/2}$$

$$\left(\frac{T_c}{T_{c0}}\right) = \left(1 + \frac{e^{-\beta_c \varepsilon_1}}{\zeta(3/2)}\right)^{-2/3}$$

$$\boxed{\left(\frac{T_c}{T_{c0}}\right) \simeq 1 - \frac{2}{3}\frac{e^{-\beta_{c0} \varepsilon_1}}{\zeta(3/2)}}$$ for small $e^{-\beta_c \varepsilon_1}$

in this term we replace $\beta_c \to \beta_{c0}$ since the difference is very small.

To see more explicitly the last step, ie that we can replace $\beta_c \to \beta_{c0}$ in the exponential term, we can do as follows

$$\frac{T_c}{T_{c0}} = 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_c \varepsilon_1} = 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_{c0}\varepsilon_1\left(\frac{T_{c0}}{T_c}\right)}$$

$$= 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_{c0}\varepsilon_1\left(1 - \frac{2}{3\zeta(3/2)} e^{-\beta_c\varepsilon_1}\right)}$$

$$= 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_{c0}\varepsilon_1} \underbrace{e^{\frac{2}{3\zeta(3/2)}\beta_{c0}\varepsilon_1 e^{-\beta_c\varepsilon_1}}}$$

where $e^{-\beta_c\varepsilon_1} \ll 1$ since $\beta_c\varepsilon_1 \gg 1$

expand. To lowest order we get $e^{\delta} \simeq 1 + \delta$

$$1 + \frac{2}{3\zeta(3/2)}\beta_{c0}\varepsilon_1 e^{-\beta_c\varepsilon_1}$$

$$\frac{T_c}{T_{c0}} \simeq 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_{c0}\varepsilon_1} - \left[\frac{2}{3\zeta(3/2)}\right]^2 e^{-\beta_{c0}\varepsilon_1} e^{-\beta_c\varepsilon_1} \beta_{c0}\varepsilon_1$$

this term is 2nd order in the small quantity $e^{-\beta_{c0}\varepsilon_1} \approx e^{-\beta_c\varepsilon_1}$

Since we previously dropped such 2nd order terms, we should drop this one too, so the leading order we get

$$\frac{T_c}{T_{c0}} \simeq 1 - \frac{2}{3\zeta(3/2)} e^{-\beta_{c0}\varepsilon_1}$$