Noninteracting Bosons of mass m & spin s

$$\langle n_{\vec{k},\sigma} \rangle = \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} \; ; \quad \varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$

$$-\infty < \mu < 0 \iff 0 < z < 1$$

Occupation of energy levels

$$\rho_0 = \underbrace{\frac{g}{V} \frac{1}{e^{-\beta\mu} - 1}}_{\rho_{GS} \text{ in ground state}} + \underbrace{\frac{g}{V} \sum_{\vec{k} \neq 0} \frac{1}{e^{\beta[\varepsilon(\vec{k}) - \mu]} - 1}}_{\rho_{ES} \text{ in excited states}}$$

$$= \frac{g}{V} \frac{z}{1 - z} + \frac{g}{\lambda^3} f^+_{3/2}(z) \; ; \quad f^+_n(z) = \frac{1}{(n-1)!} \int_0^\infty dx \, \frac{x^{n-1}}{z^{-1} e^{x} - 1}$$

For $z < 1$, $\rho_{ES}(z) < \frac{g}{\lambda^3} f^+_{3/2}(1) \equiv \rho_{ES}^{MAX} \simeq 2.612 \, g \, \lambda^3$

Canonical ensemble

$\rho_0 = \rho_{GS}(z) + \rho_{ES}(z) \Rightarrow$ eq° for z.

If $\rho_0 < \rho_{ES}^{MAX}$, $z < 1$, $\rho_0 = \underbrace{\rho_{GS}(z)}_{\xrightarrow[V \to \infty]{} 0} + \rho_{ES}(z) \underset{V \to \infty}{\simeq} \rho_{ES}(z)$

If $\rho_0 > \rho_{ES}^{MAX}$, $z \to 1$ & $\rho_{GS} = \rho_0 - \rho_{ES}^{MAX}$ finite.

True Bose Einstein condensation with a finite fraction $\alpha = \frac{\rho_{GS}}{\rho_0}$ in the ground state.

Then, $\langle n_0\rangle = \alpha V \rho_0 = \frac{g}{z^{-1}-1} \Rightarrow z^{-1} = 1 + \frac{g}{\alpha V \rho_0}$ & $z \simeq 1 - \frac{g}{\alpha V \rho_0} \xrightarrow[V\to\infty]{} 1$

Is n_0 the sole macroscopically occupied state?

$$\langle n_1\rangle = \frac{1}{z^{-1} e^{\beta\varepsilon_1} - 1} \quad ; \quad k_1 = \frac{2\pi}{L} \Rightarrow \beta\varepsilon_1 = \beta \frac{\hbar^2}{2m} \frac{4\pi^2}{L^2} = \frac{K}{L^2}$$

$$\langle n_1\rangle = \left[\left(1 + \frac{g}{\alpha L^3 \rho_0}\right)\left(1 + \frac{K}{L^2}\right) - 1\right]^{-1} \simeq \left[\frac{K}{L^2} + \frac{1}{\alpha \rho_0 L^3}\right]^{-1} \sim \frac{L^2}{K}$$

$$\rho_1 = \frac{\langle n_1\rangle}{V} \sim \frac{1}{L} \xrightarrow[V\to\infty]{} 0$$

Only the ground state has a macroscopic number of particle

Transition temperature

μ a N are not the easiest control parameter, but we can tune $\rho_{ES}^{MAX} = g \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} f_{3/2}^{+}(1)$ by changing T.

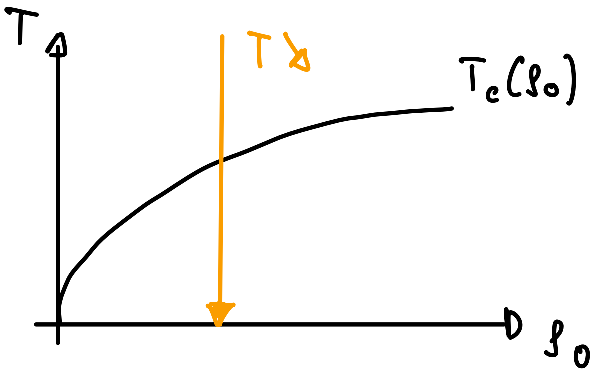
* $T > T_c$, $\rho_{ES}^{MAX} > \rho_0$, $z < 1$ & $\rho_{GS} \xrightarrow[V\to\infty]{} 0 \Rightarrow$ No BEC

* $T = T_c$, $\rho_0 = \rho_{ES}^{MAX} \Rightarrow$ $\boxed{k_B T_c = \frac{h^2}{2\pi m}\left(\frac{\rho_0}{g\, f_{3/2}^{+}(1)}\right)^{2/3}}$

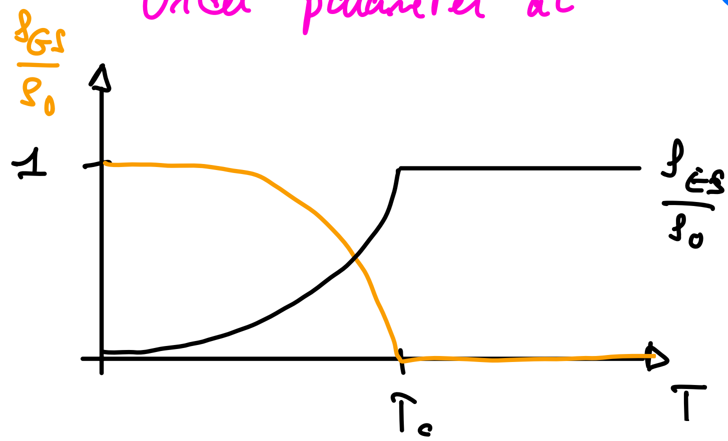
* $T < T_c$, $\rho_{GS} = \rho_0 - \underbrace{\rho_{ES}^{MAX}(T)}_{\propto T^{3/2}}$. Since $\rho_0 = \rho_{ES}^{MAX}(T_c)$, we have

$$\boxed{\frac{\rho_{GS}}{\rho_0} = 1 - \left(\frac{T}{T_c}\right)^{3/2}}$$

Phase diagram



Order parameter at



Comment: Why can we use $\rho_0 = \rho_{GS}(z) + \rho_{ES}(z)$ in the canonical ensemble while we derived it in the grand canonical ensemble?

[Crisanti, Salasnich, Sarracino, Zannetti, Arxiv: 2404.17300]

Thermodynamics

Grand potential: Treating the GS separately

$$G = k_B T g \left[\ln(1-z) + \frac{V}{(2\pi)^3} \int dk\, 4\pi k^2 \ln\left(1 - z e^{-\beta \frac{\hbar^2 k^2}{2m}}\right) \right]$$

$$x = \frac{\hbar^2 k^2}{2 m k_B T} \Rightarrow k = \sqrt{x} \sqrt{\frac{8\pi^2 m k_B T}{h^2}}$$

$$G = k_B T g \ln(1-z) + \frac{g V k_B T}{4\pi^2} \left(\frac{8\pi^2 m k_B T}{h^2} \right)^{3/2} \underbrace{\int dx\, x^{1/2} \ln(1 - z e^{-x})}_{\text{IBP} \; -\frac{2}{3} \int dx \frac{x^{3/2} z e^{-x}}{1 - z e^{-x}}}$$

$$G = k_B T g \ln(1-z) - \frac{g V k_B T}{\Lambda^3} \underbrace{\underbrace{\frac{2}{3} \frac{2}{\sqrt{\pi}}}_{\frac{1}{\frac{3}{2}!}} \int dx \frac{x^{3/2}}{z^{-1} e^{x} - 1}}_{f^+_{5/2}(z)}$$

$$\boxed{G = k_B T g \ln(1-z) - \frac{g V k_B T}{\Lambda^3} f^+_{5/2}(z)}$$

Pressure: $P = -\frac{\partial G}{\partial V} = \frac{g k_B T}{\Lambda^3} f^+_{5/2}(z)$ $\Rightarrow$ the GS bosons do not contribute to the pressure.

This makes sense: $\vec{k}_0 = 0$ so that $\vec{p}_0 = \hbar \vec{k}_0 = 0 \Rightarrow$ no momentum to transfer

$T < T_c$ $\quad P = \frac{g k_B T}{\Lambda^3} f^+_{5/2}(1) \simeq 1.31 \frac{g k_B T}{\Lambda^3} \Rightarrow$ independent from N & V!

$T > T_c$ $\quad \rho_0 \simeq \frac{g}{\Lambda^3} f^+_{3/2}(z) \Rightarrow P = \rho_0 k_B T \frac{f^+_{5/2}(z)}{f^+_{3/2}(z)}$

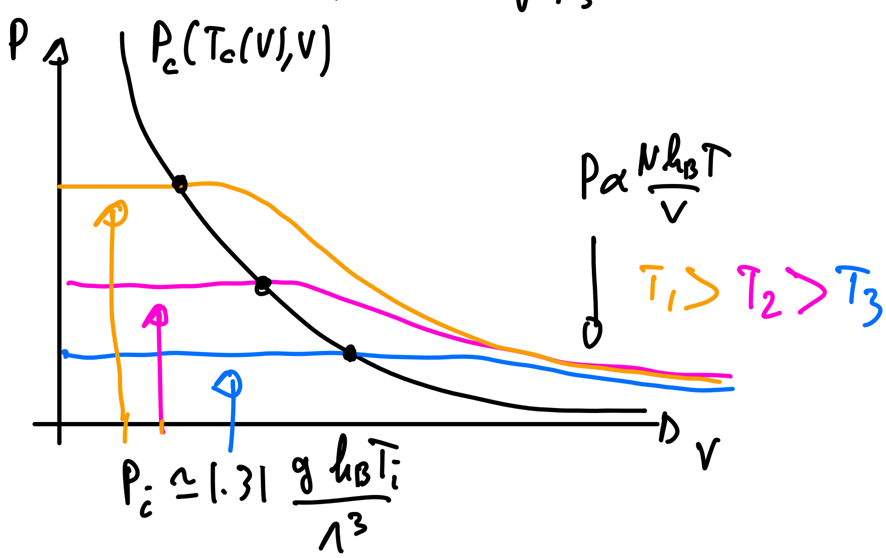
$$T \gg T_c \; ; \; z \ll 1 \, , \; f^+_m(z) = \frac{1}{(m-1)!} \int_0^\infty dx \frac{x^{m-1}}{z^{-1} e^x - 1} \simeq \frac{z}{(m-1)!} \underbrace{\int_0^\infty dx \, x^{m-1} e^{-x}}_{(m-1)!}$$

$\Rightarrow P \xrightarrow[T \gg T_c]{} \rho_0 k_B T$ as expected.

$T = T_c$ $\quad \rho_0 = \frac{N}{V} = \frac{g f^+_{3/2}(1)}{h^3} (2\pi m k_B T_c)^{3/2} \Rightarrow T_c(V) = \frac{1}{2\pi m k_B T_c} \left(\frac{N h^3}{V g f^+_{3/2}(1)} \right)^{2/3}$

$\Rightarrow$ At T_c, $P_c(T_c(V), V) \propto \frac{N T_c(V)}{V} \sim \frac{1}{V^{5/3}}$

Isotherm $P(V)$



High temperature expansion: how to connect to classical stat mech?

$f_m^+(z) \simeq z \Rightarrow$ leading order term $\Rightarrow$ what about higher orders?

$$f_m^+(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^m} \simeq z + \frac{z^2}{2^m} + \frac{z^3}{3^m} + \dots$$

$$f_m^+(z) = \frac{1}{(m-1)!}\int_0^{\infty} dx\, x^{m-1} z e^{-x} \sum_{k=0}^{\infty} (z e^{-x})^k = \frac{1}{(m-1)!}\sum_{k=0}^{\infty} z^{k+1} \underbrace{\int_0^{\infty} dx\, x^{m-1} e^{-x(1+k)}}_{\frac{(m-1)!}{(1+k)^m}}$$

$u = x(1+k)$

From here $\Rightarrow$ P as a series in z, ρ_0 as a series in z $\Big\} \Rightarrow P$ as a series in ρ_0.

Energy & heat capacity:

$$\langle E \rangle = \partial_\beta(\beta G) = \frac{3gV}{\Lambda^4} f_{5/2}^+(z)\,\frac{\partial \Lambda}{\partial \beta} \quad ; \Lambda = \sqrt{\frac{h^2\beta}{2\pi m}} \Rightarrow \partial_\beta \Lambda = \frac{k_B T}{2}\Lambda$$

$$\langle E \rangle = \frac{3}{2} k_B T \frac{gV}{\Lambda^3} f_{5/2}^+(z) = \frac{3}{2} PV$$

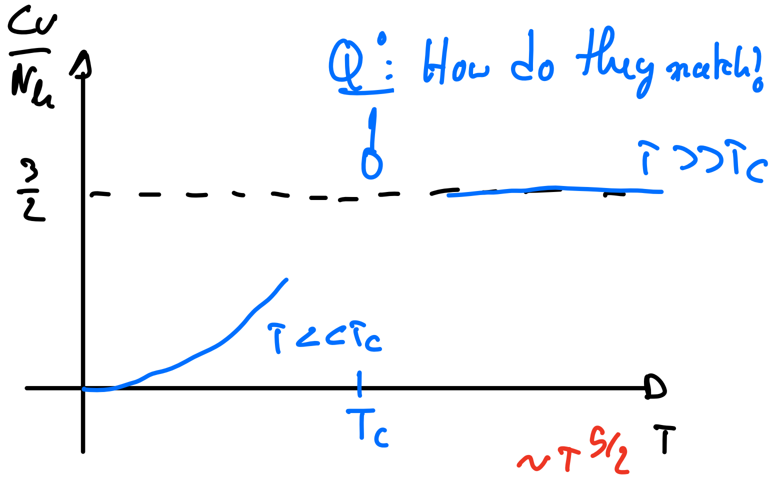
Low temperature limit

$T > T_c$, $\rho_{GS} = 0$ & $N \underset{V\to\infty}{\simeq} \frac{gV}{\Lambda^3} f_{3/2}^+(z) \Rightarrow E = \frac{3}{2} N k_B T \frac{f_{5/2}^+(z)}{f_{3/2}^+(z)}$

$T \gg T_c$ leads to $E \simeq \frac{3}{2} N k_B T$ & $C_V = \frac{3}{2}N$.

$T = T_c$, $\rho_0 = \frac{g}{\Lambda_c^3} f_{3/2}^+(1)$ & $gV = \frac{N\Lambda_c^3}{f_{3/2}^+(1)}$

$T < T_c$, $\langle E \rangle = \frac{3}{2} N k_B T \left(\frac{\Lambda_c}{\Lambda}\right)^3 \frac{f_{5/2}^+(1)}{f_{3/2}^+(1)} \propto N T^{5/2} \Rightarrow C_V \propto T^{3/2} N$



$$T > T_c \; ; \; \langle E \rangle = \frac{3}{2} k_B \overbrace{T \frac{gV}{\lambda^3}}^{\sim T^{5/2}} f^+_{5/2}(z)$$

$$C_V = \frac{3}{2} k_B T \frac{gV}{\lambda^3} \left[\frac{5}{2T} f^+_{5/2}(z) + \underbrace{\frac{\partial z}{\partial T}}_{(2)} \cdot \underbrace{\frac{\partial}{\partial z} f^+_{5/2}(z)}_{(1)} \right]$$

(1) Direct algebra $\partial_z f^+_m = \frac{1}{z} f^+_{m-1}$

$$\frac{\partial}{\partial z} \int_0^\infty dx \frac{x^{m-1}}{z^{-1}e^x - 1} = -\int_0^\infty dx \frac{x^{m-1}}{(z^{-1}e^x-1)^2}\left(-\frac{1}{z^2}e^x\right) = \frac{1}{z}\int_0^\infty dx \overbrace{\frac{z^{-1}e^x}{(z^{-1}e^x-1)^2}}^{= \frac{\partial}{\partial x}\left[-\frac{1}{z^{-1}e^x-1}\right]} x^{m-1}$$

$$\overset{\text{IBP}}{=} \frac{m-1}{z} \int_0^\infty dx \frac{x^{m-2}}{z^{-1}e^x - 1}$$

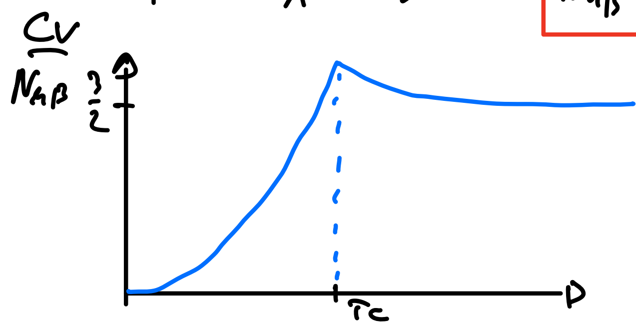
Multiplying both sides by $\frac{1}{m!}$ leads to $\partial_z f^+_m = \frac{1}{z} f^+_{m-1}$

(2) $\rho_0 \lambda^3 = g f^+_{3/2}(z) \Rightarrow \frac{\partial}{\partial T} \ln(\rho_0 \lambda^3) = -\frac{3}{2T} = \frac{\partial_T f^+_{3/2}(z)}{f^+_{3/2}(z)} = \frac{1}{z} \frac{f^+_{1/2}(z)}{f^+_{3/2}(z)} \frac{\partial z}{\partial T}$

$$\Rightarrow \frac{\partial z}{\partial T} = -\frac{3z}{2T} \frac{f^+_{1/2}(z)}{f^+_{3/2}(z)}$$

$$① + ② \Rightarrow \boxed{C_V = \frac{15}{4} k_B \frac{gV}{\Lambda^3} f^+_{5/2}(z) - \frac{9}{4} k_B \frac{gV}{\Lambda^3} \frac{f^+_{3/2}(z)^2}{f^+_{1/2}(z)}}$$

As $T \to T_c$,
$$\left.\begin{aligned} f^+_{5/2} &\to 1.34 \\ f^+_{3/2} &\to 2.61 \\ f^+_{1/2} &\to \infty \end{aligned}\right\} \quad C_V \to \frac{15}{4} k_B \overbrace{\frac{gV}{\Lambda^3}}^{N/f^+_{3/2}(1)} f^+_{5/2}(1) \quad \& \quad \boxed{\frac{C_V}{Nk_B} \simeq 1.92 > \frac{3}{2}}$$



High temperature expansions: The approach to $T = T_c$ ($T > T_c$) relies on a high-T expansion, which leads to

$$\frac{C_V}{Nk_B} \simeq \frac{3}{2}\left(1 + \rho_0 \frac{\Lambda^3}{2^{7/2}} + \dots\right) \geq \frac{3}{2}$$